Hole-spin qubits in silicon and germanium quantum dots

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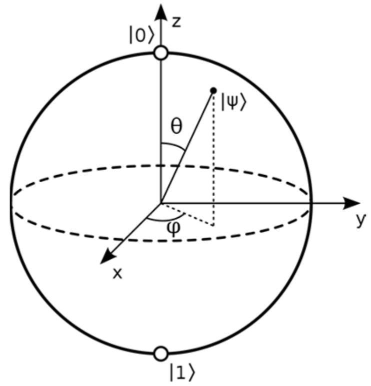
https://www.iqubits.eu/

Introduction

Qubit: two-state QM system, basic unit of quantum information

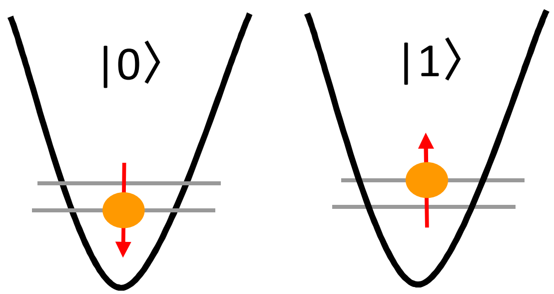
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$|\alpha|^2 + |\beta|^2 = 1$$



Operations:

- Initialization in a known state;
- Manipulation through quantum logic gates;
- Measurement.



Spin qubits: realized with the «spins» of localized charge carriers

Example of two-qubit gate: Loss-Di Vincenzo proposal

- Double quantum dot (two coupled dots);
- No magnetic field;
- Time-dependent exchange interaction.

Initialization: state 0 in dot 1 and state 1 in dot 2, high barrier between the dots

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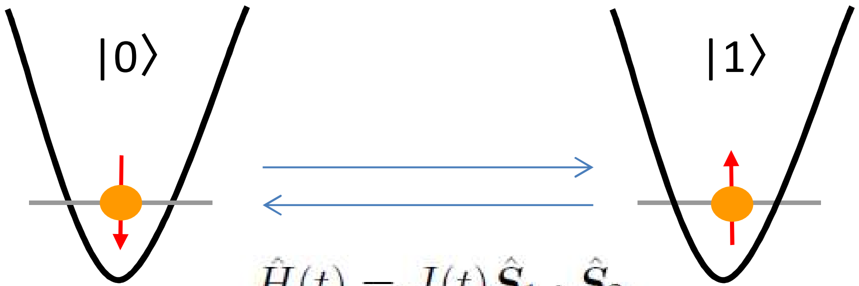

$$\hat{H}(t) = J(t)\hat{S}_1 \cdot \hat{S}_2$$

Manipulation: barrier pulsed to low voltage in a time-dependent way

Example of two-qubit gate: Loss-Di Vincenzo proposal

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After some time: qubit states have been swapped (SWAP gate)

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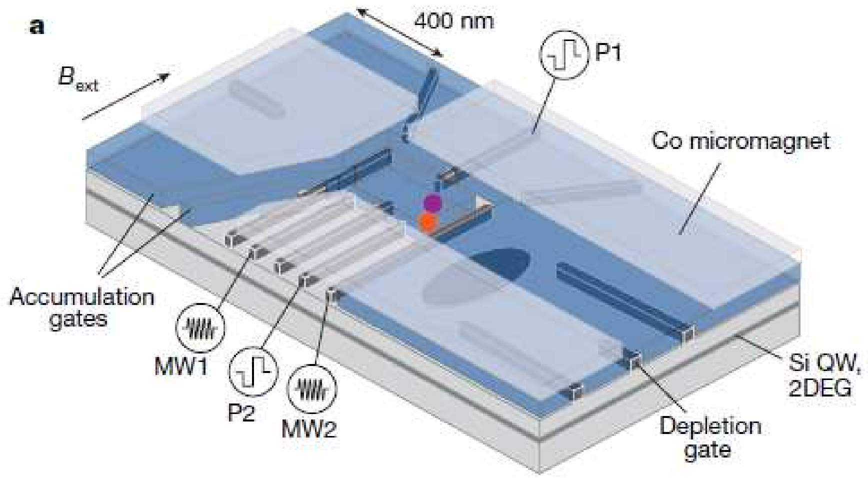
Sqrt(SWAP) + single-qubit gates → universal quantum computation

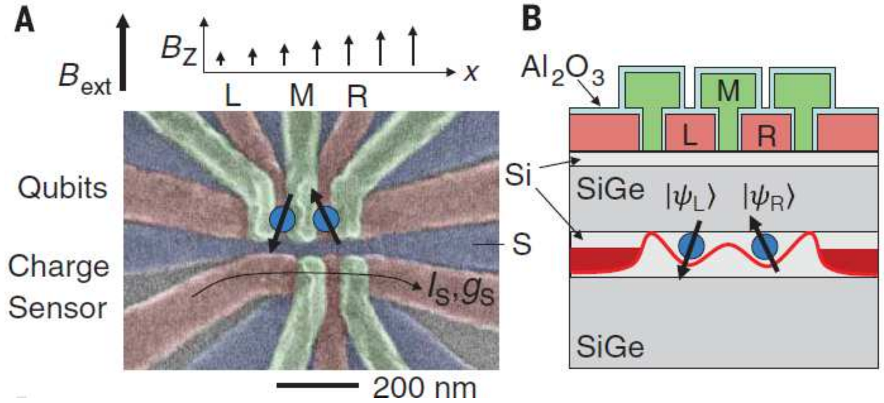
Why silicon and germanium? Why holes?

Why silicon and germanium? Why holes?

- High natural abundance of non-magnetic isotopes (^{28}Si + ^{30}Si > 95% and ^{70}Ge + ^{72}Ge + ^{74}Ge + ^{76}Ge > 92%) + isotopic purification → small hyperfine interaction → long coherence times

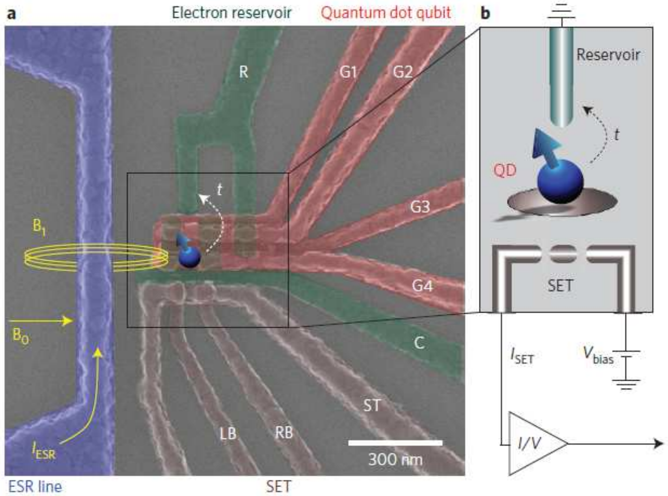


T. F. Watson et al., Nature **555,** 633 (2018)

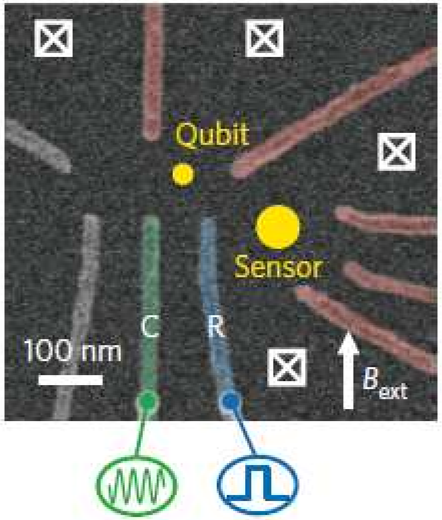


D. M. Zajac et al., Science **359,** 439 (2018)

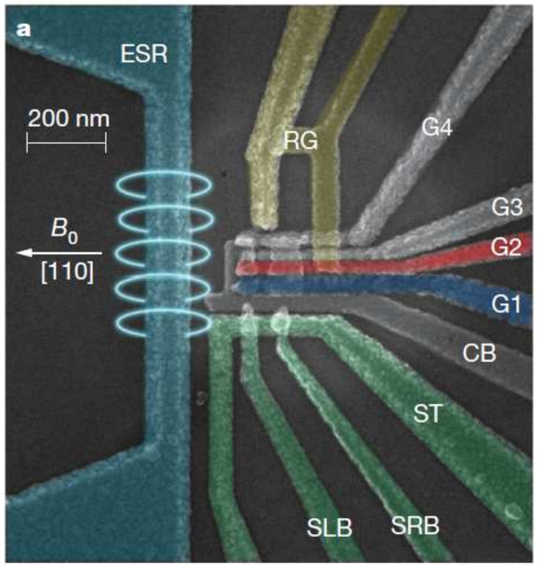
- High degree of control of single and few charge carriers in Si and Ge QDs achieved experimentally during the last decade (gates and readout)



M. Veldhorst et al., Nature Nanotech. **9,** 981 (2014)

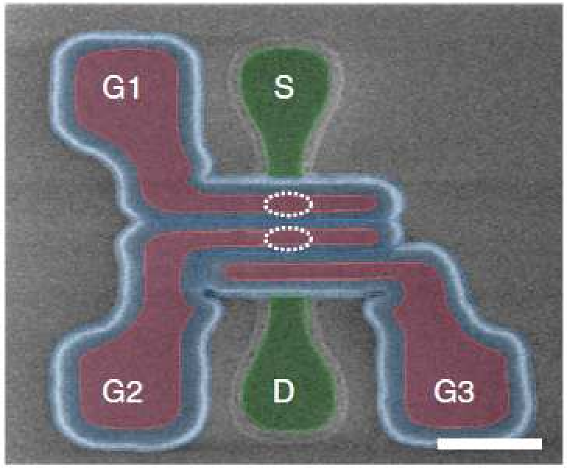


J. Yoneda et al., Nature Nanotech. **13,** 102 (2018)

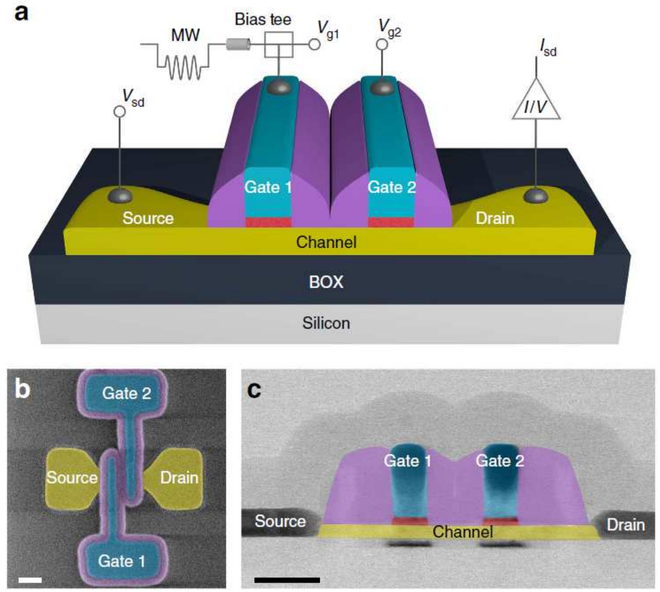


W. Huang et al., Nature **569,** 532 (2019)

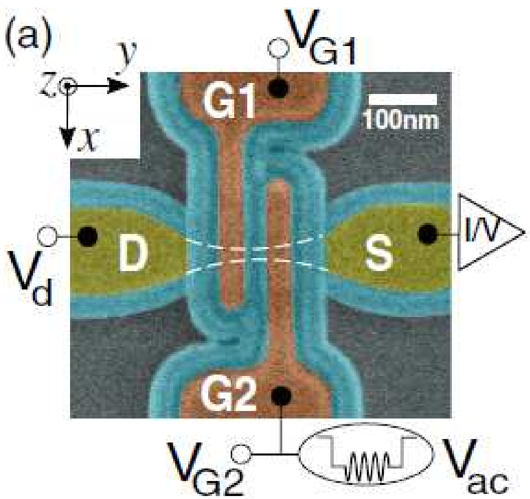
- Key materials for modern electronics → well-established industrial fabrication techniques → integration of qubits and control circuits (CMOS qubits)



M. Urdampilleta et al., Nature Nanotech. **14,** 737 (2019)

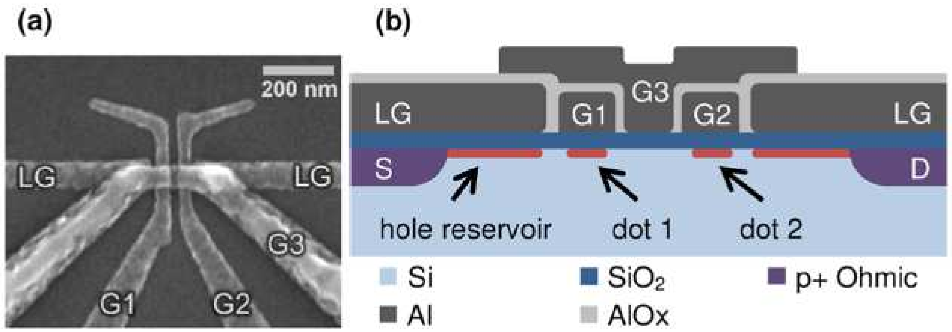


R. Maurand et al., Nature Commun. **7,** 13575 (2016)

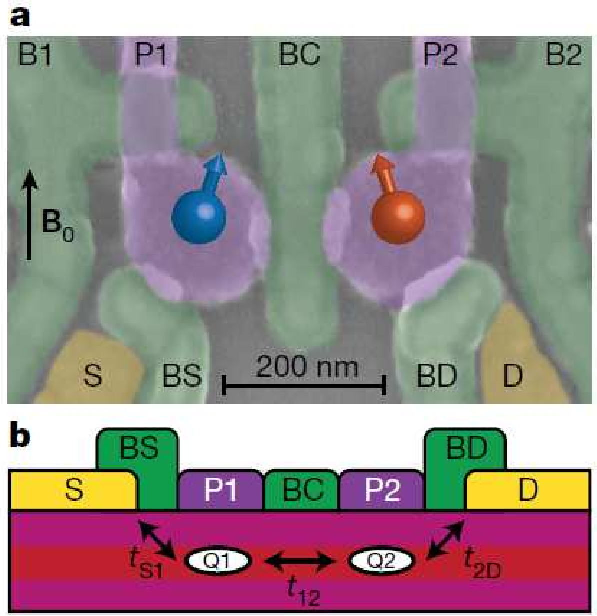


A. Crippa et al., Phys. Rev. Lett. **120,** 137702 (2018)

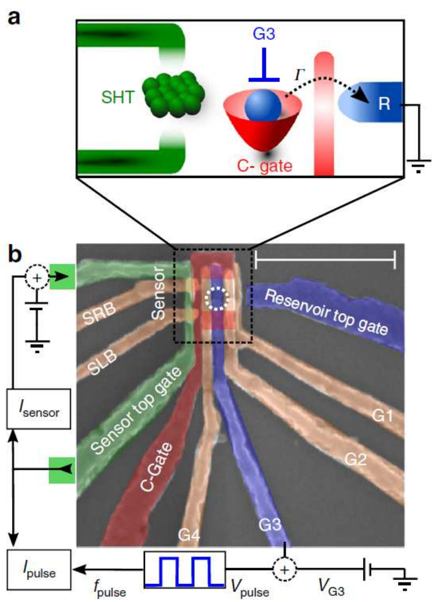
- Valence band made of *p* orbitals → further reduction of hyperfine interaction and larger spin-orbit coupling w. r. to conduction band → hole-spin qubits can be manipulated fully *electrically*



R. Li et al., Nano Lett. **15,** 7314 (2015)



N. W. Hendrickx et al., Nature **577,** 487 (2020)



S. D. Liles et al., Nature Commun. **9,** 3255 (2018)

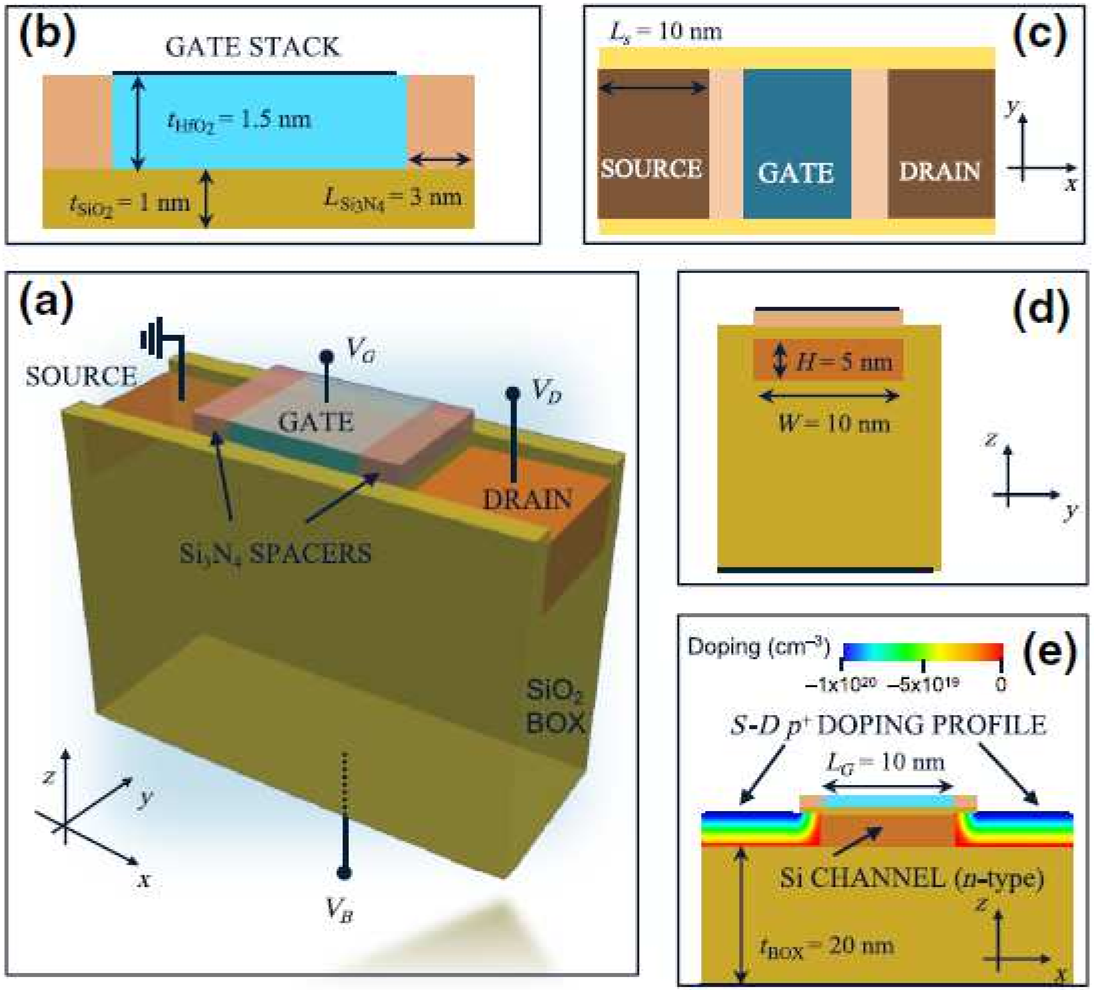
Main challenge

Need to operate the qubit at **millikelvin temperatures** to enhance coherence times; need to operate the control electronics at **1-4 K** to allow for a sufficiently fast removal of dissipated power → conflicting requirements

Qubit implementation in down-scaled MOSFETs (high quantum confinement → higher excitation energies → possibility of operating the qubit at higher temperatures)

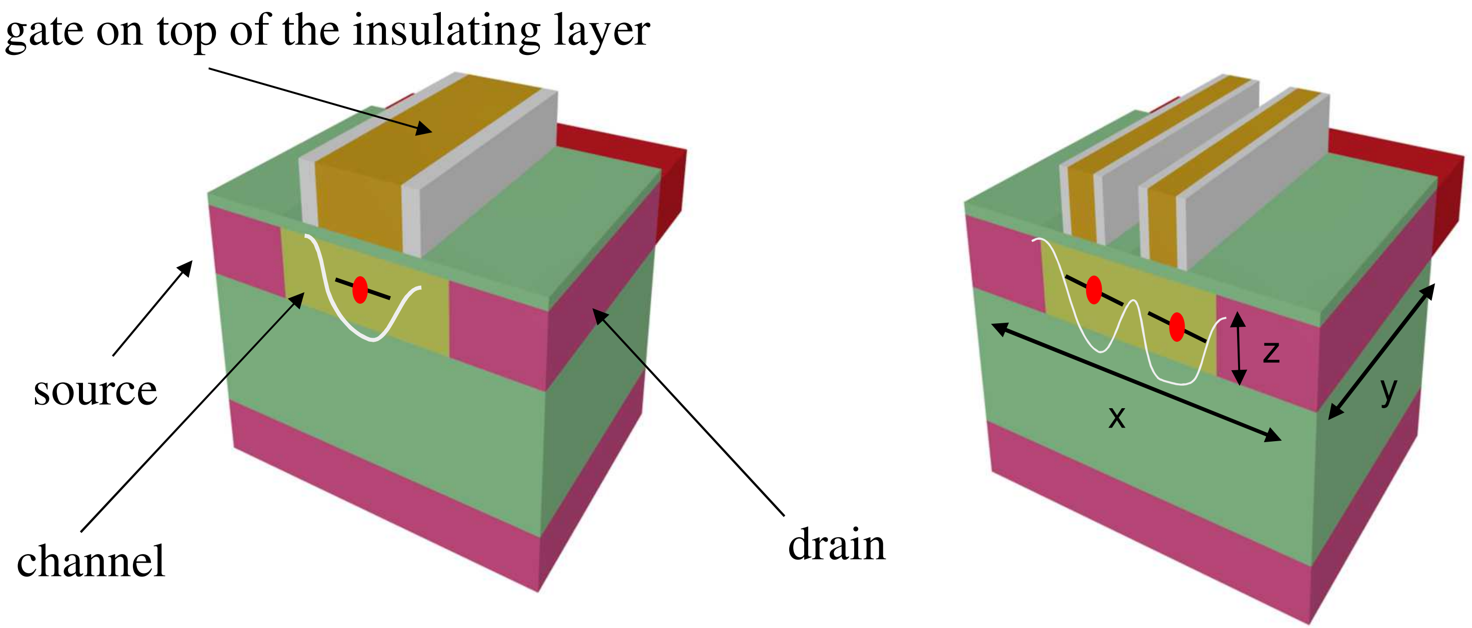
Scaled Si *p*MOSFET (scaled version of GlobalFoundries 22-nm FDSOI process)

Qubit manipulation through voltage pulses applied to the top gate



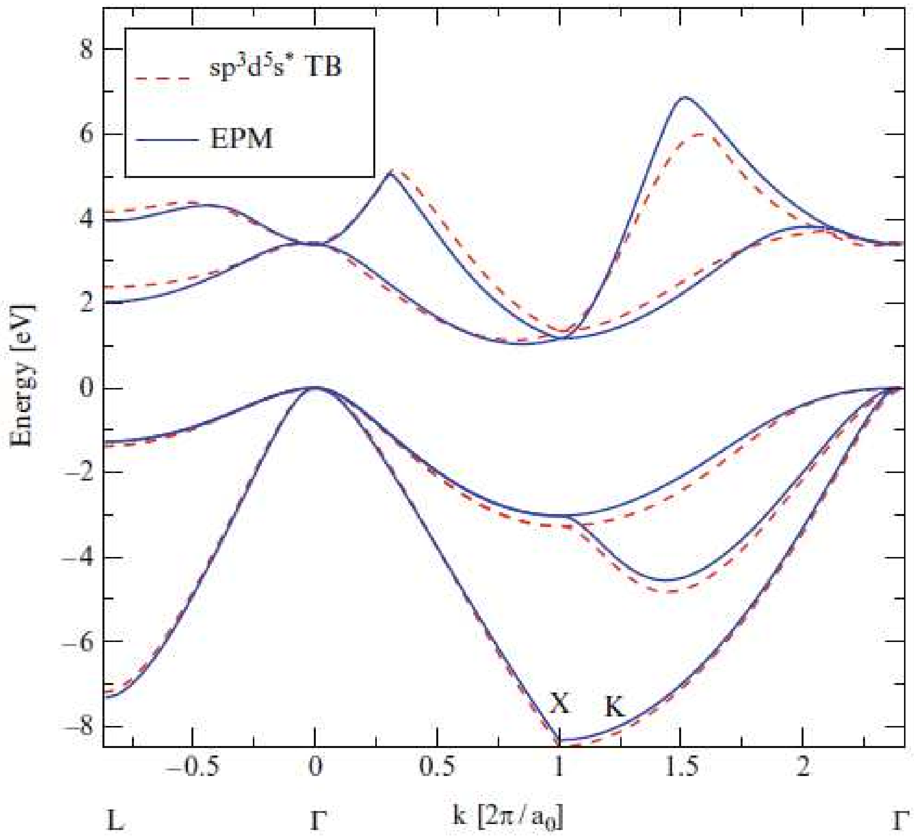
L. Bellentani et al., Phys. Rev. Applied **16,** 054034 (2021)

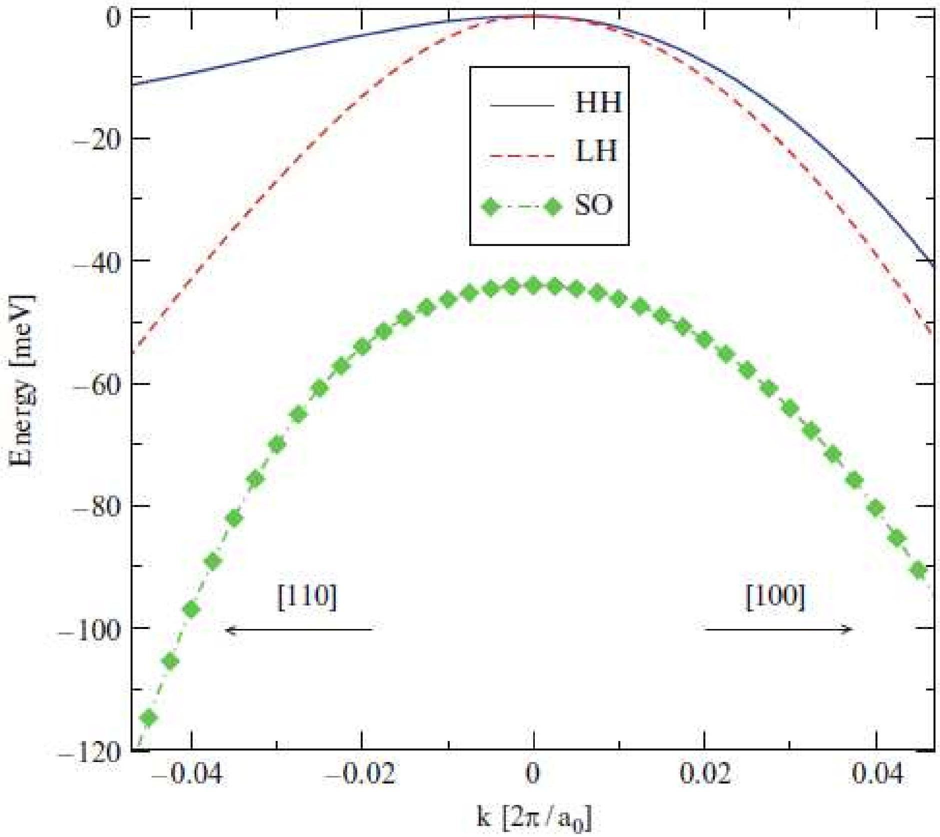
Application of one or more gates to generate single or multiple QD confinement potential inside the Si channel



→ Goal: Investigate the feasibility of one-hole or two-hole qubits in single or double quantum dots

Holes at the Γ point





- The unit cell of Si and Ge contains two atoms
- Three *p* orbitals are relevant for the valence bands at their maximum point (Γ)
- Six Bloch spin-orbital states needed to describe holes at Γ: $j = 3/2$ and $j = 1/2$ multiplets
- $j = 3/2$ and $|m| = 3/2$: heavy holes; $j = 3/2$ and $|m| = 1/2$: light holes; $j = 1/2$: split-off bands

- Including confinement (QD): envelope function scheme

basis $\{|\tfrac{3}{2},\tfrac{3}{2}\rangle, |\tfrac{3}{2},\tfrac{1}{2}\rangle, |\tfrac{3}{2},-\tfrac{1}{2}\rangle, |\tfrac{3}{2},-\tfrac{3}{2}\rangle, |\tfrac{1}{2},\tfrac{1}{2}\rangle, |\tfrac{1}{2},-\tfrac{1}{2}\rangle\}$

$$\mathcal{H}_{\boldsymbol{k},\boldsymbol{r}} = \begin{pmatrix} P_{\boldsymbol{k}}+Q_{\boldsymbol{k}}+V_{\boldsymbol{r}} & -S_{\boldsymbol{k}} & \widetilde{R}_{\boldsymbol{k}} & 0 & -\frac{1}{\sqrt{2}}S_{\boldsymbol{k}} & \sqrt{2}\widetilde{R}_{\boldsymbol{k}} \\ -S_{\boldsymbol{k}}^{\dagger} & P_{\boldsymbol{k}}-Q_{\boldsymbol{k}}+V_{\boldsymbol{r}} & 0 & \widetilde{R}_{\boldsymbol{k}} & -\sqrt{2}Q_{\boldsymbol{k}} & \sqrt{\frac{3}{2}}S_{\boldsymbol{k}} \\ \widetilde{R}_{\boldsymbol{k}}^{\dagger} & 0 & P_{\boldsymbol{k}}-Q_{\boldsymbol{k}}+V_{\boldsymbol{r}} & S_{\boldsymbol{k}} & \sqrt{\frac{3}{2}}S_{\boldsymbol{k}}^{\dagger} & \sqrt{2}Q_{\boldsymbol{k}} \\ 0 & \widetilde{R}_{\boldsymbol{k}}^{\dagger} & S_{\boldsymbol{k}}^{\dagger} & P_{\boldsymbol{k}}+Q_{\boldsymbol{k}}+V_{\boldsymbol{r}} & -\sqrt{2}\widetilde{R}_{\boldsymbol{k}}^{\dagger} & -\frac{1}{\sqrt{2}}S_{\boldsymbol{k}}^{\dagger} \\ -\frac{1}{\sqrt{2}}S_{\boldsymbol{k}}^{\dagger} & -\sqrt{2}Q_{\boldsymbol{k}} & \sqrt{\frac{3}{2}}S_{\boldsymbol{k}} & -\sqrt{2}\widetilde{R}_{\boldsymbol{k}} & P_{\boldsymbol{k}}+\Delta+V_{\boldsymbol{r}} & 0 \\ \sqrt{2}\widetilde{R}_{\boldsymbol{k}}^{\dagger} & \sqrt{\frac{3}{2}}S_{\boldsymbol{k}}^{\dagger} & \sqrt{2}Q_{\boldsymbol{k}} & -\frac{1}{\sqrt{2}}S_{\boldsymbol{k}} & 0 & P_{\boldsymbol{k}}+\Delta+V_{\boldsymbol{r}} \end{pmatrix}$$

- Diagonalization yields the 6-component envelope function:

$$\psi_{\nu,B}(\boldsymbol{r})$$

eigenstate

6-valued band index $B = (j, m)$

Inter- and intra-band interactions

- Two-hole states are obtained via the Configuration-Interaction (CI) method
- Two-body matrix elements of the interaction are required

Textbook expression:

$$V_{\{\nu\}} = \int d\boldsymbol{r} \int d\boldsymbol{r}' \, \psi^*_{\nu_1}(\boldsymbol{r}) \, \psi^*_{\nu_2}(\boldsymbol{r}') \, V_{\text{Coulomb}}(\boldsymbol{r} - \boldsymbol{r}') \, \psi_{\nu_3}(\boldsymbol{r}') \, \psi_{\nu_4}(\boldsymbol{r})$$

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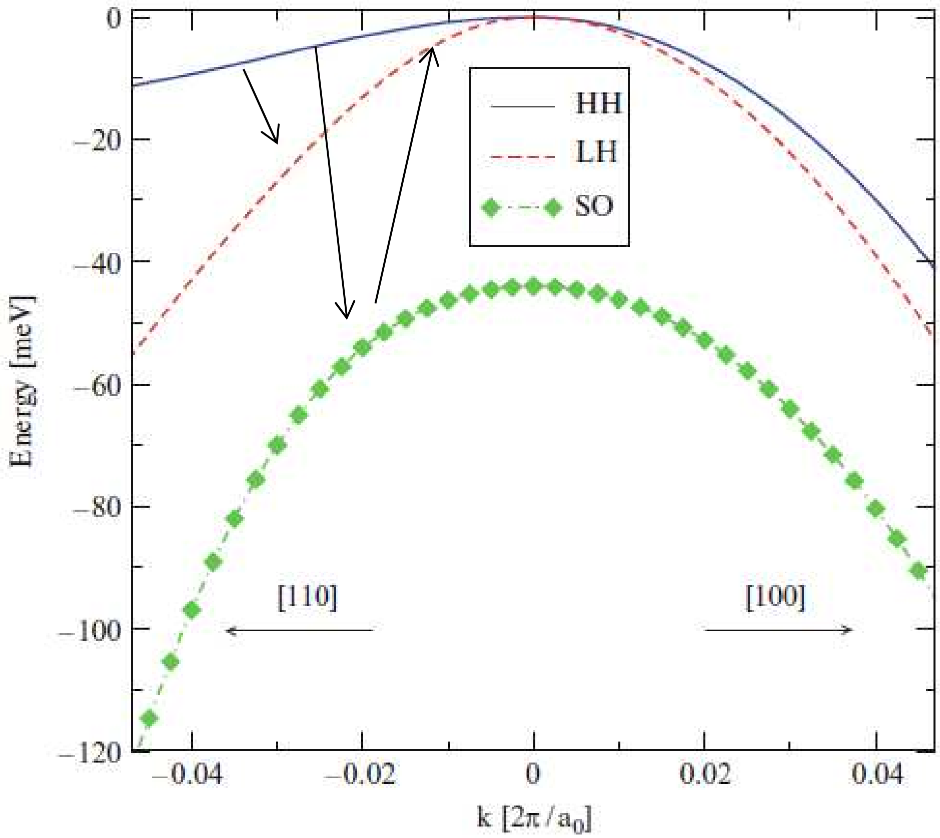
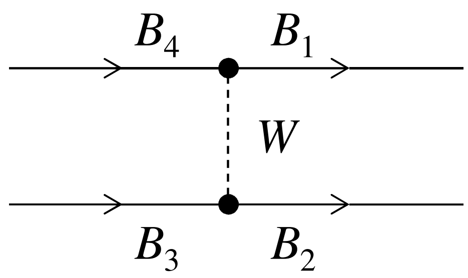
BUT we are dealing with a multi-band system:

$$V_{\{\nu\}} = \sum_{\{B\}} \int d\boldsymbol{r} \int d\boldsymbol{r}' \, \psi^*_{\nu_1,B_1}(\boldsymbol{r}) \, \psi^*_{\nu_2,B_2}(\boldsymbol{r}') \, W_{B_1,B_2,B_3,B_4}(\boldsymbol{r}-\boldsymbol{r}') \, \psi_{\nu_3,B_3}(\boldsymbol{r}') \, \psi_{\nu_4,B_4}(\boldsymbol{r})$$

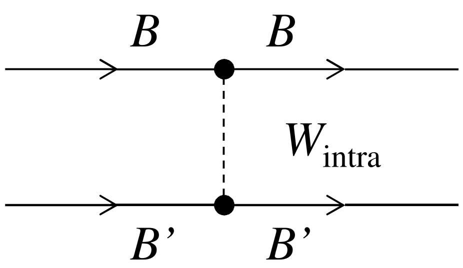
Band-dependent interaction

A. Secchi et al., Phys. Rev. B **104,** 205409 (2021)

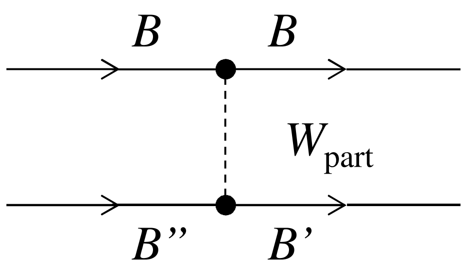




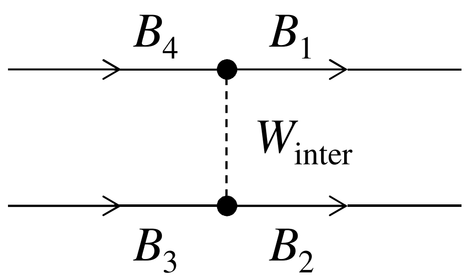
Intraband (36)

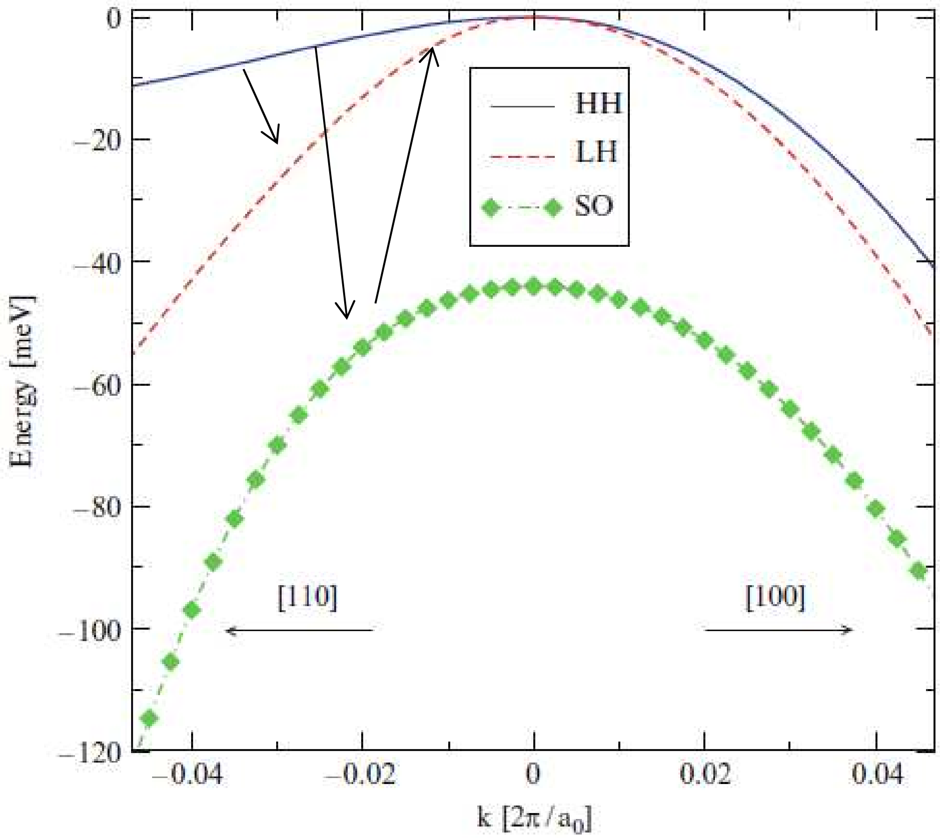


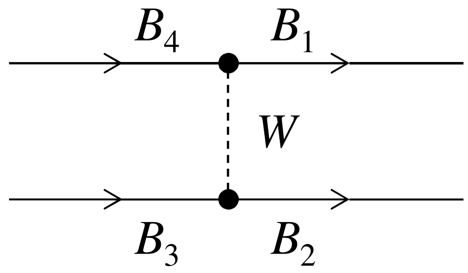
Partially interband (32)



Interband (120)

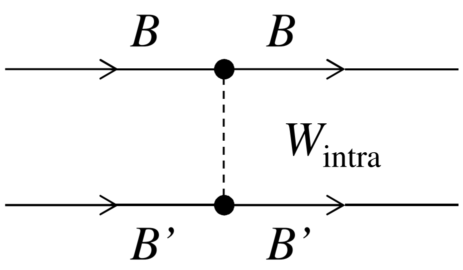




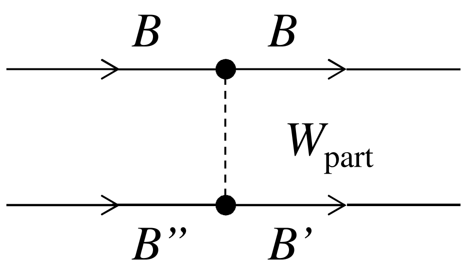


Short-ranged
Relevant for downscaled devices

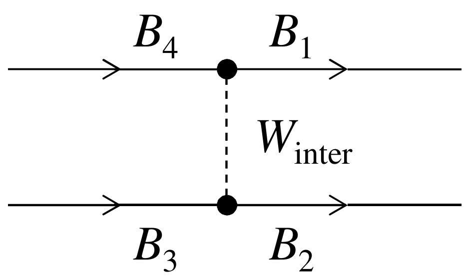
Intraband (36)



Partially interband (32)

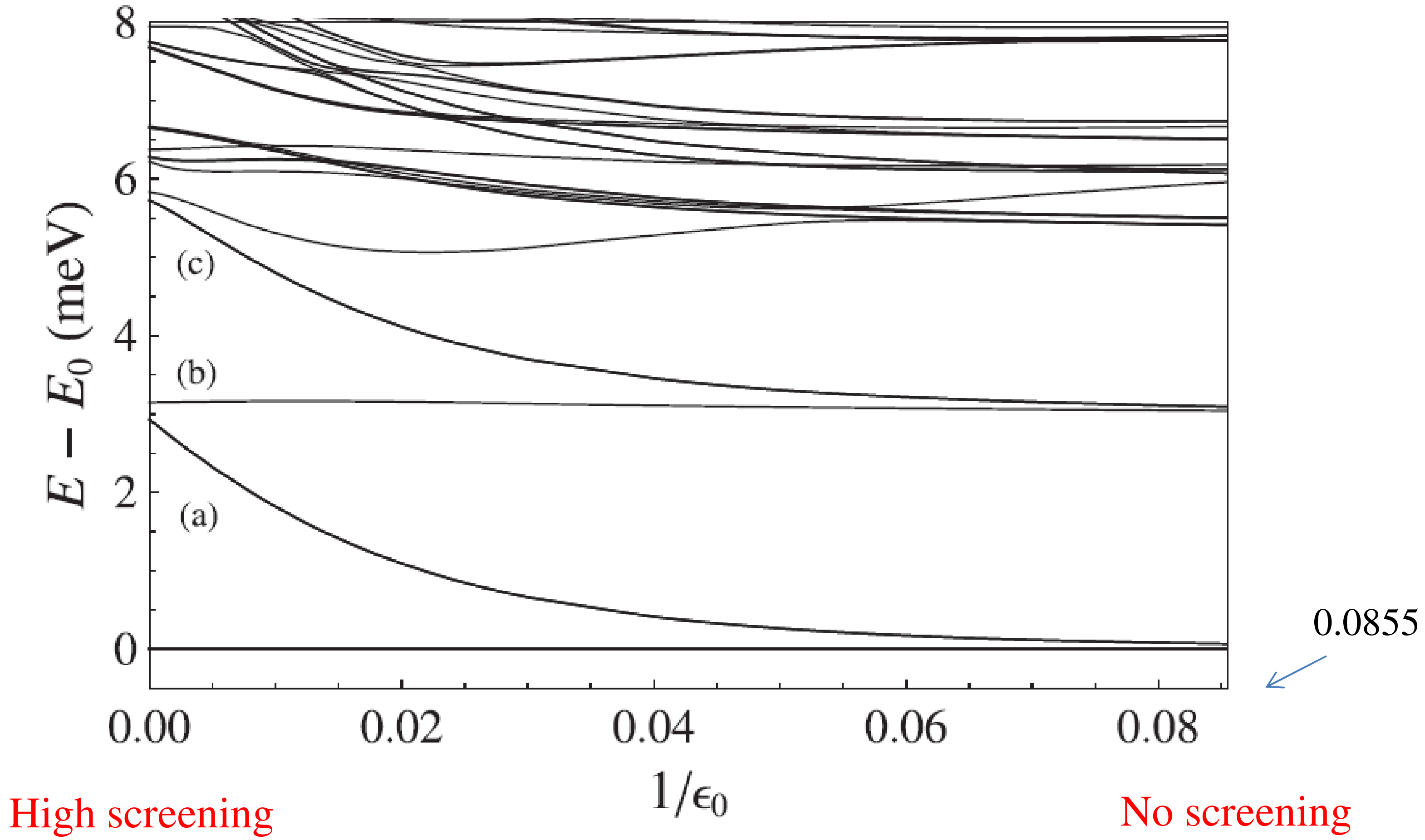


Interband (120)



Single quantum dot, two-hole excitation energies

$$V_{QD}(\boldsymbol{r}) = \frac{1}{2}(\kappa_x x^2 + \kappa_y y^2 + \kappa_z z^2) \qquad \boldsymbol{\ell} = (10, 4, 2)\ \mathrm{nm}$$



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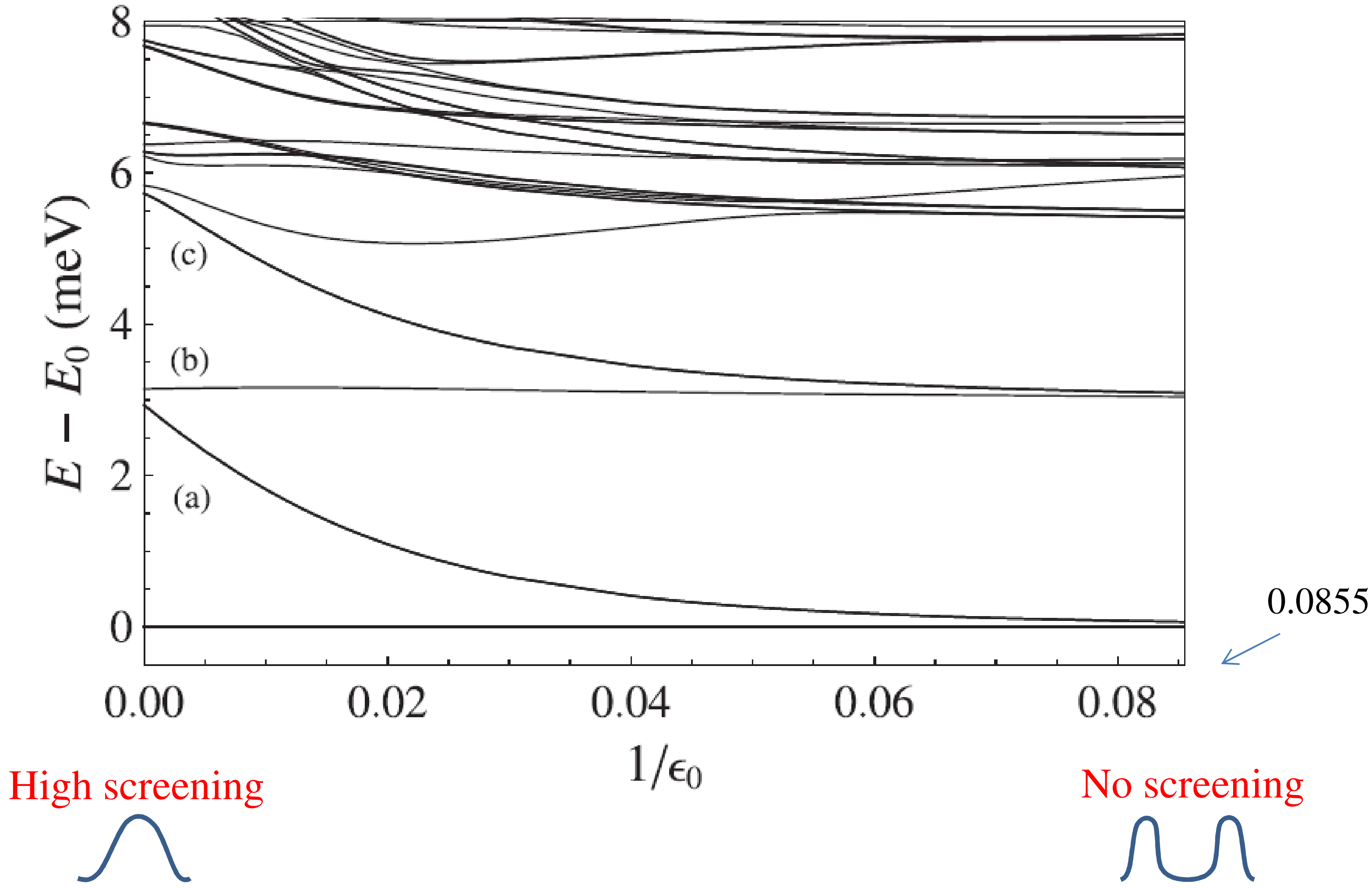

Recap (1)

- 6-band envelope-function formalism;
- Configuration-Interaction (CI) method for interacting two-hole systems;
- Intra- and inter-band Coulomb scattering processes;
- Interband Coulomb processes are relevant in a regime of high screening and/or strong confinement;
- In unscreened Si single quantum dots → two-hole Wigner molecules.

PHYSICAL REVIEW B **104**, 205409 (2021)

Inter- and intraband Coulomb interactions between holes in silicon nanostructures

Andrea Secchi,* Laura Bellentani, Andrea Bertoni, and Filippo Troiani
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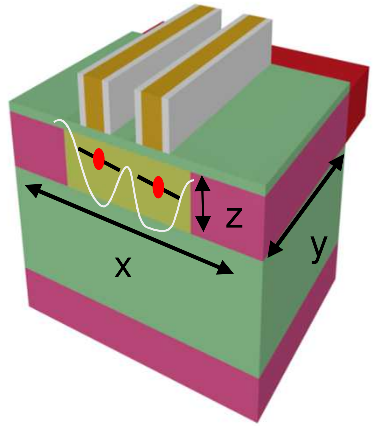
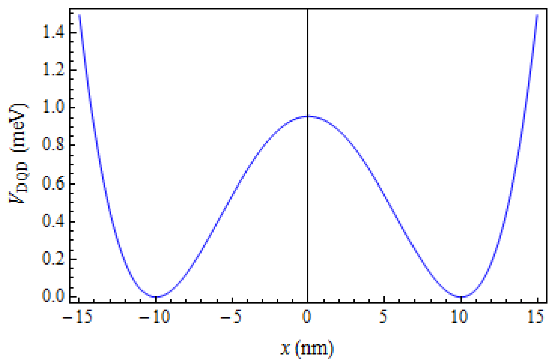
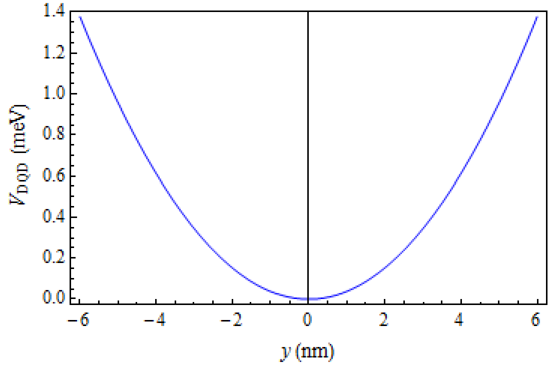
Double quantum dots

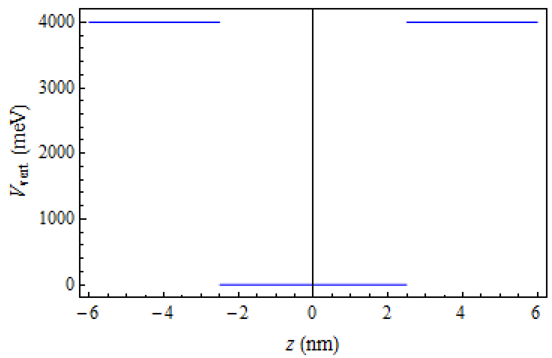


Two-qubit gates via exchange modulation
(Loss-Di Vincenzo proposal)

$$V(\boldsymbol{r}) = V_{\mathrm{DQD}}(x) + V_{\mathrm{QD}}(y) + V_{\parallel}\theta(|z| - L_z/2)$$







$$V_{\mathrm{DQD}}(x) = \frac{1}{2}\kappa\frac{(x^2 - a^2)^2}{4a^2} \qquad V_{\mathrm{QD}}(y) = \frac{1}{2}\kappa y^2 \qquad V_{\parallel}\theta(|z| - L_z/2)$$

→ approximations of realistic potentials computed with TCAD or Poisson simulations

→ weak tunneling regime

A. Secchi et al., Phys. Rev. B **104,** 035302 (2021)

Single-hole states

Denoted as $|\psi_\alpha\rangle$

Because of time-reversal symmetry in the absence of a magnetic field, they are organized in Kramers doublets:

$$e_1 = e_2\,, \quad e_3 = e_4\,, \quad \ldots\,, \quad e_{2n+1} = e_{2n+2}$$

General form:

$$|\psi_\alpha\rangle = \sum_b |\psi_{\alpha,b}\rangle \otimes |b\rangle$$

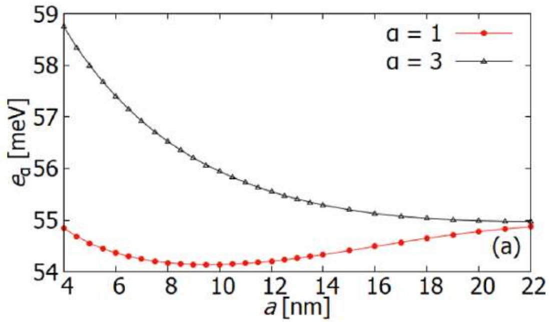
band-dependent envelope function

band spinor (Bloch state)
$b = (j, m)$

This state *cannot* be factorized exactly as:

$$\left|\psi_\alpha^{\text{fact}}\right\rangle \equiv |\psi_{\alpha,1}\rangle \otimes \sum_b c_{\alpha,b}|b\rangle$$

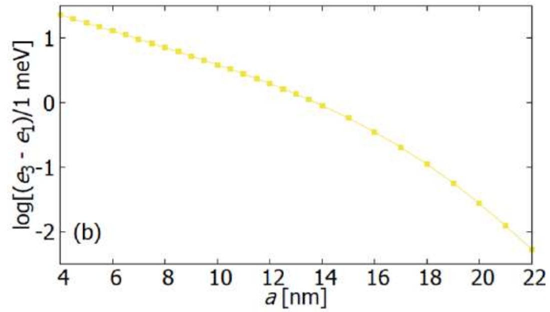
«Spin»-orbital correlation: the population is distributed among different bands and the envelope functions corresponding to different bands are not parallel



Si

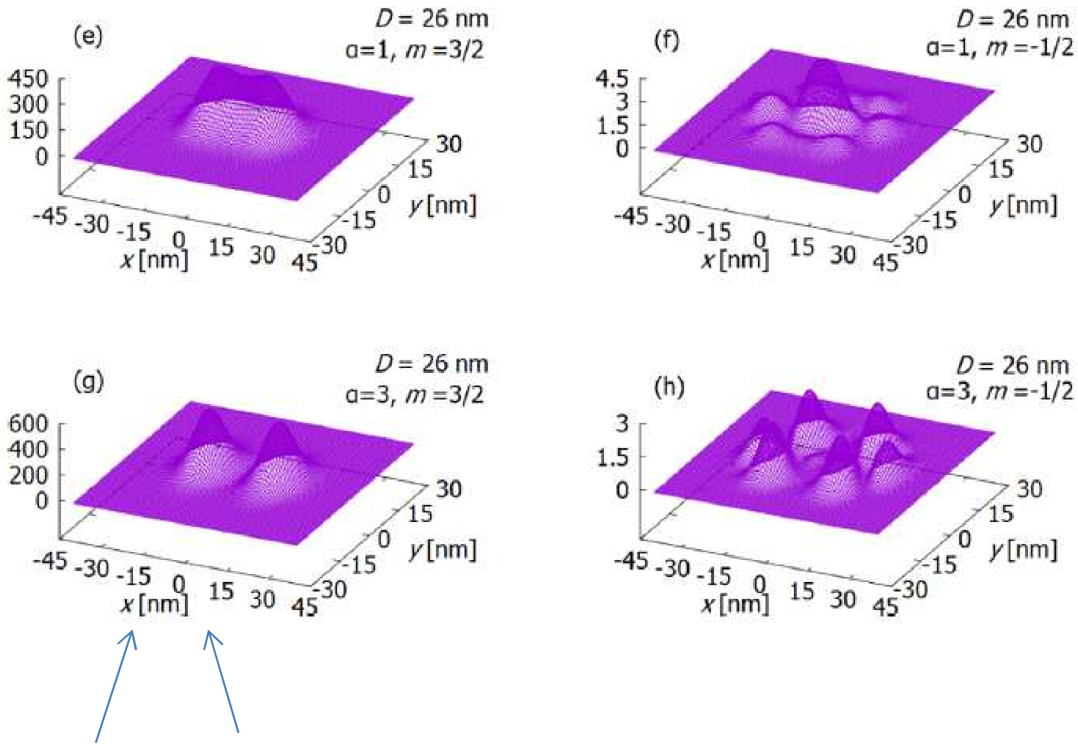
Si requires shorter interdot distances than Ge (larger effective masses)

→ it is relevant to study the impact of strain



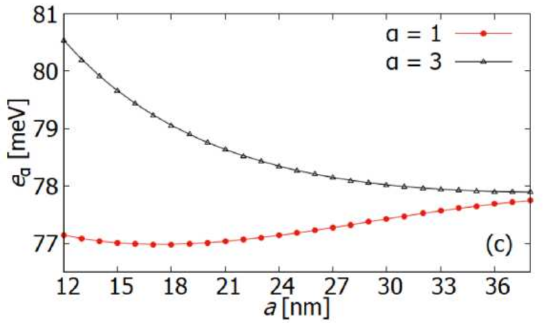
Si

Si

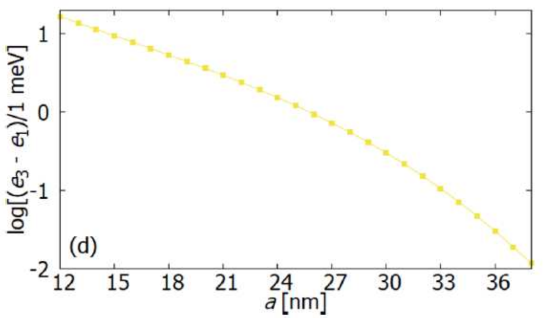


Dot 1

Dot 2



Ge



Ge

Band compositions and mirror symmetry

Si	$\|\psi_1\rangle$		$\|\psi_3\rangle$	
a (nm)	4	22	4	22
$p_{\alpha,3/2,3/2}$	0.989	0.904	0.895	0.919
$p_{\alpha,3/2,-1/2}$	0.006	0.0801	0.083	0.0643
$\langle\sigma_{yz}\rangle_\alpha$	0.996	1.00	−0.973	−1.00

$$\langle x,y,z|\sigma_{yz}|\psi_\alpha\rangle = \psi_\alpha(-x,y,z)$$

$$\langle\sigma_{yz}\rangle_\alpha = \sum_b \int dr\, \psi^*_{\alpha,b}(x,y,z)\,\psi_{\alpha,b}(-x,y,z)$$

- The heavy-hole component is dominant, followed by a small light-hole component; the split-off band is negligible → small entanglement
- Single-particle states are close to being eigenstates of the mirror symmetry operators (with even or odd parity)
- Results for Ge are analogous; the heavy-hole weight is even larger

Two-hole states

General form: combination of Slater determinants

$$|\Psi_k\rangle = \sum_{\alpha,\beta} C^k_{\alpha\beta}|\Phi_{\alpha\beta}\rangle \qquad \text{where} \quad |\Phi_{\alpha\beta}\rangle = \frac{1}{\sqrt{2}}\left(|\psi_\alpha\rangle|\psi_\beta\rangle - |\psi_\beta\rangle|\psi_\alpha\rangle\right)$$

neglect split-off bands: each hole has $j = 3/2$ (heavy and light holes)

(J, M) representation (eigenstates of square modulus and third component of total angular momentum):

$$|\Psi_k\rangle = \sum_{J,M} \underbrace{|\psi_{k,J,M}\rangle}_{\text{2-hole orbitals}} \otimes \underbrace{|J,M\rangle}_{\text{2-hole spinors}} \quad \text{where} \quad \begin{array}{l} J \in \{0,1,2,3\} \\ M \in \{-J,-J+1,\ldots,J\} \end{array} \quad \text{(16 spinors)}$$

spinor weigths $\quad p_{k,J,M} = \langle\psi_{k,J,M}|\psi_{k,J,M}\rangle$

<u>Main messages from the numerics</u>

- Lowest energy states: singlet and triplet

- Complicated spinor structure

- The singlet-triplet gap decreases with *a* faster than the single-particle gap

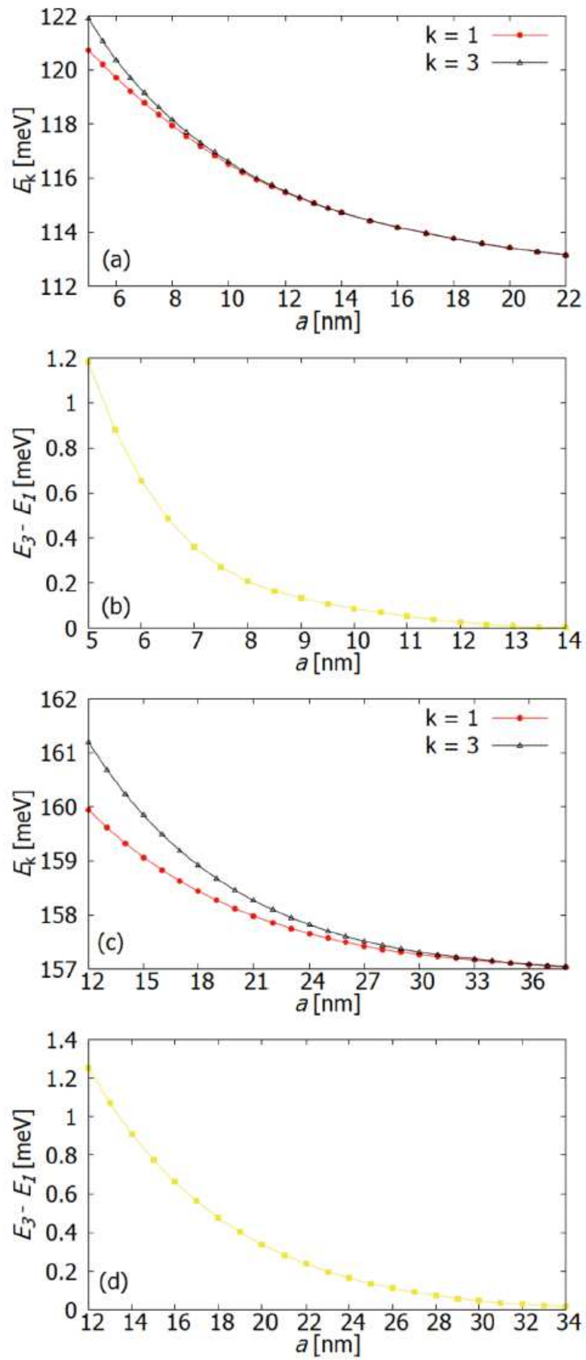
- The singlet-triplet gap is significantly larger for Ge at the same *a*

Si

Si

Ge

Ge



Spinor compositions

(relevant for external field coupling and decoherence)

Si	S ($k=1$)		T_0 ($k=3$)	
a (nm)	5	14	5	14
$p_{k,0,0}$	0.490	0.487	0.000	0.000
$p_{k,2,0}$	0.477	0.488	0.000	0.006
$p_{k,2,\pm2}$	0.012	0.001	0.008	0.012
$p_{k,1,0}$	0.000	0.000	0.860	0.878
$p_{k,3,0}$	0.000	0.000	0.099	0.098
$p_{k,3,\pm2}$	0.004	0.005	0.012	0.005
Ge	S ($k=1$)		T_0 ($k=3$)	
a (nm)	12	34	12	34
$p_{k,0,0}$	0.499	0.499	0.000	0.000
$p_{k,2,0}$	0.499	0.499	0.000	0.000
$p_{k,2,\pm2}$	0.000	0.000	0.000	0.000
$p_{k,1,0}$	0.000	0.000	0.897	0.898
$p_{k,3,0}$	0.000	0.000	0.100	0.100
$p_{k,3,\pm2}$	0.000	0.000	0.000	0.000

minority-symmetry terms (anti-symmetric spinors)

minority-symmetry terms (symmetric spinors)

Effective 4-band Hubbard model

Motivation: better understanding of physics + possible extension to large arrays of qubits

$$\hat{H}_{\mathrm{DQD}} = \hat{H}_{k\cdot p} + \underbrace{\hat{V}_1 + \hat{V}_2 + \hat{V}_{12}}_{\hat{V}_{\mathrm{DQD}}}$$

Localized single-dot single-particle states:

$$(\hat{H}_{k\cdot p} + \hat{V}_s)|\psi_{s,\tau}\rangle = E_{s,\tau}|\psi_{s,\tau}\rangle$$

s = site index
τ = Kramers spin

Numerical calculations on the single-dots suggest the following approximation:

$$|\psi_{s,\Uparrow}\rangle \equiv |\psi_{s,H}\rangle \otimes \left(\left|\tfrac{3}{2}\right\rangle + \left|-\tfrac{3}{2}\right\rangle\right) + |\psi_{s,L}\rangle \otimes \left(\left|\tfrac{1}{2}\right\rangle + \left|-\tfrac{1}{2}\right\rangle\right)$$
$$|\psi_{s,\Downarrow}\rangle \equiv |\psi^*_{s,H}\rangle \otimes \left(\left|\tfrac{3}{2}\right\rangle - \left|-\tfrac{3}{2}\right\rangle\right) - |\psi^*_{s,L}\rangle \otimes \left(\left|\tfrac{1}{2}\right\rangle - \left|-\tfrac{1}{2}\right\rangle\right)$$

We derive the effective model Hamiltonian

$$\hat{H}_{\mathrm{Hubbard}} = [T(\hat{\psi}^\dagger_{1,\Uparrow}\hat{\psi}_{2,\Uparrow} + \hat{\psi}^\dagger_{2,\Downarrow}\hat{\psi}_{1,\Downarrow}) + \mathrm{H.c.}]$$
$$+ U(\hat{n}_{1,\Uparrow}\hat{n}_{1,\Downarrow} + \hat{n}_{2,\Uparrow}\hat{n}_{2,\Downarrow}),$$

and we solve it for $N = 1$ and 2, comparing the solutions with the numerical results.

Solution for $N = 1$

Eigenenergies (both doubly degenerate): $e_{\pm} = \pm |T|$ NB: $T = |T| e^{i\theta}$

Eigenstates: $|\psi_{\pm,\tau}\rangle = \frac{1}{\sqrt{2}}(\hat{\psi}^{\dagger}_{1,\tau} \pm e^{-i\theta}\,\hat{\psi}^{\dagger}_{2,\tau})|0\rangle$

Expansion on the *m* basis:

$$
\begin{aligned}
|\psi_{\pm,\Uparrow}\rangle = \frac{1}{\sqrt{2}}\Bigg[& (|\psi_{1,H}\rangle \pm e^{-i\theta}|\psi_{2,H}\rangle) \otimes \left(\left|\frac{3}{2}\right\rangle + \left|-\frac{3}{2}\right\rangle\right) \\
& + (|\psi_{1,L}\rangle \pm e^{-i\theta}|\psi_{2,L}\rangle) \otimes \left(\left|\frac{1}{2}\right\rangle + \left|-\frac{1}{2}\right\rangle\right)\Bigg], \\
|\psi_{\pm,\Downarrow}\rangle = \frac{1}{\sqrt{2}}\Bigg[& (|\psi^{*}_{1,H}\rangle \pm e^{-i\theta}|\psi^{*}_{2,H}\rangle) \otimes \left(\left|\frac{3}{2}\right\rangle - \left|-\frac{3}{2}\right\rangle\right) \\
& - (|\psi^{*}_{1,L}\rangle \pm e^{-i\theta}|\psi^{*}_{2,L}\rangle) \otimes \left(\left|\frac{1}{2}\right\rangle - \left|-\frac{1}{2}\right\rangle\right)\Bigg].
\end{aligned}
$$

Solution for $N = 1$

Eigenenergies (both doubly degenerate): $e_{\pm} = \pm|T|$ NB: $T = |T|e^{i\theta}$

Eigenstates: $|\psi_{\pm,\tau}\rangle = \frac{1}{\sqrt{2}}(\hat{\psi}^{\dagger}_{1,\tau} \pm e^{-i\theta}\,\hat{\psi}^{\dagger}_{2,\tau})|0\rangle$

Expansion on the *m* basis:

$$|\psi_{\pm,\Uparrow}\rangle = \frac{1}{\sqrt{2}}\Bigg[(|\psi_{1,H}\rangle \pm e^{-i\theta}|\psi_{2,H}\rangle) \otimes \left(\left|\frac{3}{2}\right\rangle + \left|-\frac{3}{2}\right\rangle\right)$$

$$+ (|\psi_{1,L}\rangle \pm e^{-i\theta}|\psi_{2,L}\rangle) \otimes \left(\left|\frac{1}{2}\right\rangle + \left|-\frac{1}{2}\right\rangle\right)\Bigg],$$

m mixing

$$|\psi_{\pm,\Downarrow}\rangle = \frac{1}{\sqrt{2}}\Bigg[(|\psi^{*}_{1,H}\rangle \pm e^{-i\theta}|\psi^{*}_{2,H}\rangle) \otimes \left(\left|\frac{3}{2}\right\rangle - \left|-\frac{3}{2}\right\rangle\right)$$

$$- (|\psi^{*}_{1,L}\rangle \pm e^{-i\theta}|\psi^{*}_{2,L}\rangle) \otimes \left(\left|\frac{1}{2}\right\rangle - \left|-\frac{1}{2}\right\rangle\right)\Bigg].$$

Solution for $N = 1$

Eigenenergies (both doubly degenerate): $e_\pm = \pm|T|$ NB: $T = |T|e^{i\theta}$

Eigenstates: $|\psi_{\pm,\tau}\rangle = \frac{1}{\sqrt{2}}(\hat{\psi}^\dagger_{1,\tau} \pm e^{-i\theta}\hat{\psi}^\dagger_{2,\tau})|0\rangle$

Expansion on the *m* basis:

Spatial (anti)-symmetry for real *T* consistent with numerical results

$$
\begin{aligned}
|\psi_{\pm,\Uparrow}\rangle = \frac{1}{\sqrt{2}}\Bigg[&(|\psi_{1,H}\rangle \pm e^{-i\theta}|\psi_{2,H}\rangle) \otimes \left(\left|\frac{3}{2}\right\rangle + \left|-\frac{3}{2}\right\rangle\right) \\
&+ (|\psi_{1,L}\rangle \pm e^{-i\theta}|\psi_{2,L}\rangle) \otimes \left(\left|\frac{1}{2}\right\rangle + \left|-\frac{1}{2}\right\rangle\right)\Bigg], \\
|\psi_{\pm,\Downarrow}\rangle = \frac{1}{\sqrt{2}}\Bigg[&(|\psi^*_{1,H}\rangle \pm e^{-i\theta}|\psi^*_{2,H}\rangle) \otimes \left(\left|\frac{3}{2}\right\rangle - \left|-\frac{3}{2}\right\rangle\right) \\
&- (|\psi^*_{1,L}\rangle \pm e^{-i\theta}|\psi^*_{2,L}\rangle) \otimes \left(\left|\frac{1}{2}\right\rangle - \left|-\frac{1}{2}\right\rangle\right)\Bigg].
\end{aligned}
$$

m mixing

Solution for $N = 2$

We directly consider the Heisenberg-Hamiltonian limit (low T/U):

$$\hat{H}_{\text{Heisenberg}} = J\left(\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 - \tfrac{1}{4}\right) \qquad \text{where} \quad \hat{\boldsymbol{S}}_s = \frac{1}{2} \sum_{\tau,\tau' \in \{\Uparrow,\Downarrow\}} \hat{\psi}^\dagger_{s,\tau} \boldsymbol{\sigma}_{\tau,\tau'} \hat{\psi}_{s,\tau'}$$

(Kramers-spin operator for site s)

Eigenstates:

$$|\mathbb{S}\rangle \equiv \frac{1}{\sqrt{2}}(\hat{\psi}^\dagger_{1,\Uparrow}\hat{\psi}^\dagger_{2,\Downarrow} - \hat{\psi}^\dagger_{1,\Downarrow}\hat{\psi}^\dagger_{2,\Uparrow})|0\rangle$$

Energy = - J

$$\left.\begin{aligned}
|\mathbb{T}_\Uparrow\rangle &\equiv \hat{\psi}^\dagger_{1,\Uparrow}\hat{\psi}^\dagger_{2,\Uparrow}|0\rangle \\
|\mathbb{T}_0\rangle &\equiv \frac{1}{\sqrt{2}}(\hat{\psi}^\dagger_{1,\Uparrow}\hat{\psi}^\dagger_{2,\Downarrow} + \hat{\psi}^\dagger_{1,\Downarrow}\hat{\psi}^\dagger_{2,\Uparrow})|0\rangle \\
|\mathbb{T}_\Downarrow\rangle &\equiv \hat{\psi}^\dagger_{1,\Downarrow}\hat{\psi}^\dagger_{2,\Downarrow}|0\rangle
\end{aligned}\right\} \quad \text{Energy} = 0$$

Expansion of the singlet state on the (J, M) basis:

$$\begin{aligned}
|\mathbb{S}\rangle = &\left(\left|\Psi^{S}_{1H,2H}\right\rangle + \left|\Psi^{S}_{1L,2L}\right\rangle\right) \otimes |0, 0\rangle \\
&+ \left(\left|\Psi^{S}_{1H,2H}\right\rangle - \left|\Psi^{S}_{1L,2L}\right\rangle\right) \otimes |2, 0\rangle \\
&+ \frac{1}{\sqrt{2}}\left(\left|\Psi^{S}_{1L,2H}\right\rangle + \left|\Psi^{S}_{1H,2L}\right\rangle\right) \otimes (|2, 2\rangle + |2, -2\rangle) \\
&+ \frac{1}{\sqrt{2}}\left(\left|\Psi^{A}_{1L,2H}\right\rangle - \left|\Psi^{A}_{1H,2L}\right\rangle\right) \otimes (|3, 2\rangle - |3, -2\rangle)
\end{aligned}$$

Expansion of the singlet state on the (J, M) basis:

Antisymmetric spinors

$$
\begin{aligned}
|\mathbb{S}\rangle = {} & \left(\left|\Psi^S_{1H,2H}\right\rangle + \left|\Psi^S_{1L,2L}\right\rangle\right) \otimes |0, 0\rangle \\
& + \left(\left|\Psi^S_{1H,2H}\right\rangle - \left|\Psi^S_{1L,2L}\right\rangle\right) \otimes |2, 0\rangle \\
& + \frac{1}{\sqrt{2}}\left(\left|\Psi^S_{1L,2H}\right\rangle + \left|\Psi^S_{1H,2L}\right\rangle\right) \otimes \left(|2, 2\rangle + |2, -2\rangle\right) \\
& + \frac{1}{\sqrt{2}}\left(\left|\Psi^A_{1L,2H}\right\rangle - \left|\Psi^A_{1H,2L}\right\rangle\right) \otimes \left(|3, 2\rangle - |3, -2\rangle\right)
\end{aligned}
$$

Symmetric spinors

Expansion of the singlet state on the (J, M) basis:

Antisymmetric spinors

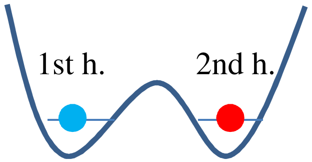
Symmetric orbitals

$$
\begin{aligned}
|\mathbb{S}\rangle = & \left(\left|\Psi^{S}_{1H,2H}\right\rangle + \left|\Psi^{S}_{1L,2L}\right\rangle\right) \otimes |0,0\rangle \\
& + \left(\left|\Psi^{S}_{1H,2H}\right\rangle - \left|\Psi^{S}_{1L,2L}\right\rangle\right) \otimes |2,0\rangle \\
& + \frac{1}{\sqrt{2}}\left(\left|\Psi^{S}_{1L,2H}\right\rangle + \left|\Psi^{S}_{1H,2L}\right\rangle\right) \otimes \left(|2,2\rangle + |2,-2\rangle\right) \\
& + \frac{1}{\sqrt{2}}\left(\left|\Psi^{A}_{1L,2H}\right\rangle - \left|\Psi^{A}_{1H,2L}\right\rangle\right) \otimes \left(|3,2\rangle - |3,-2\rangle\right)
\end{aligned}
$$

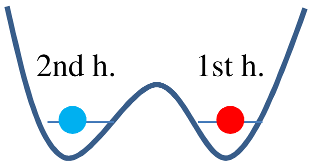
Antisymmetric orbitals
(L-H mixing and non-parallelism
is necessary)

Symmetric spinors

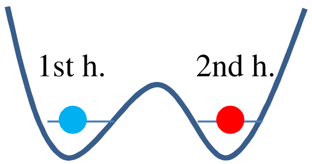
$\left|\Psi^{S}_{1L,2H}\right\rangle =$



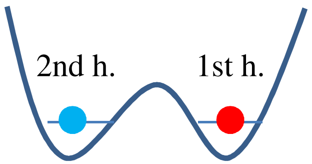
$+$



$\left|\Psi^{A}_{1L,2H}\right\rangle =$



$-$



Expansion of the singlet state on the (J, M) basis:

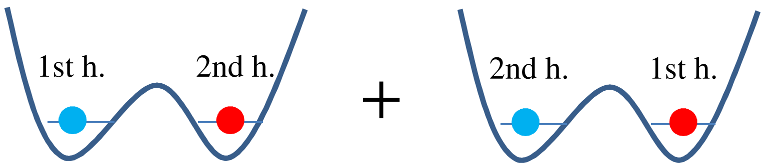
Antisymmetric spinors

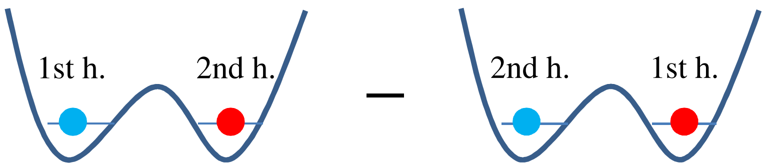
$$
\begin{aligned}
|\mathbb{S}\rangle = &\left(\left|\Psi^S_{1H,2H}\right\rangle + \left|\Psi^S_{1L,2L}\right\rangle\right) \otimes |0,0\rangle \\
&+ \left(\left|\Psi^S_{1H,2H}\right\rangle - \left|\Psi^S_{1L,2L}\right\rangle\right) \otimes |2,0\rangle \\
&+ \frac{1}{\sqrt{2}}\left(\left|\Psi^S_{1L,2H}\right\rangle + \left|\Psi^S_{1H,2L}\right\rangle\right) \otimes \left(|2,2\rangle + |2,-2\rangle\right) \\
&+ \frac{1}{\sqrt{2}}\left(\left|\Psi^A_{1L,2H}\right\rangle - \left|\Psi^A_{1H,2L}\right\rangle\right) \otimes \left(|3,2\rangle - |3,-2\rangle\right)
\end{aligned}
$$

Symmetric orbitals

Antisymmetric orbitals
(L-H mixing and non-parallelism
is necessary)

Symmetric spinors

$\left|\Psi^S_{1L,2H}\right\rangle =$ 

$\left|\Psi^A_{1L,2H}\right\rangle =$ 

Singlet in the 2-band,
spin-1/2 case:

$$|S\rangle = \left|\Psi^S_{1,2}\right\rangle \otimes |0,0\rangle$$

Expansion of a triplet state on the (J, M) basis:

$$
\begin{aligned}
|T_{z,+}\rangle &= \sqrt{2}\,\left|\Psi^{A}_{1H,2H}\right\rangle \otimes |3,3\rangle \\
&+ \sqrt{2}\,\left|\Psi^{A}_{1L,2L}\right\rangle \otimes \left(\sqrt{\frac{2}{5}}\,|1,-1\rangle + \sqrt{\frac{3}{5}}\,|3,-1\rangle\right) \\
&+ \left(\left|\Psi^{A}_{1L,2H}\right\rangle + \left|\Psi^{A}_{1H,2L}\right\rangle\right) \otimes \left(\sqrt{\frac{3}{5}}\,|1,1\rangle \right. \\
&\left. - \sqrt{\frac{2}{5}}\,|3,1\rangle\right) + \left(\left|\Psi^{S}_{1L,2H}\right\rangle - \left|\Psi^{S}_{1H,2L}\right\rangle\right) \otimes |2,1\rangle,
\end{aligned}
$$

Symmetric spinors

Antisymmetric orbitals

Symmetric orbital
(L-H mixing and non-parallelism
is necessary)

Antisymmetric spinor

Analogous triplet state in
the 2-band, spin-1/2 case:

$$|T_{\uparrow\uparrow}\rangle = \left|\Psi^{A}_{1,2}\right\rangle \otimes |1,1\rangle$$

Expansion of a triplet state on the (J, M) basis:

$$
\begin{aligned}
|T_{z,+}\rangle &= \sqrt{2}\,\left|\Psi^A_{1H,2H}\right\rangle \otimes |3, 3\rangle \\
&+ \sqrt{2}\,\left|\Psi^A_{1L,2L}\right\rangle \otimes \left(\sqrt{\frac{2}{5}}\,|1, -1\rangle + \sqrt{\frac{3}{5}}\,|3, -1\rangle\right) \\
&+ \left(\left|\Psi^A_{1L,2H}\right\rangle + \left|\Psi^A_{1H,2L}\right\rangle\right) \otimes \left(\sqrt{\frac{3}{5}}\,|1, 1\rangle\right. \\
&\left. - \sqrt{\frac{2}{5}}\,|3, 1\rangle\right) + \left(\left|\Psi^S_{1L,2H}\right\rangle - \left|\Psi^S_{1H,2L}\right\rangle\right) \otimes |2, 1\rangle,
\end{aligned}
$$

Symmetric spinors

Antisymmetric orbitals

Symmetric orbital
(L-H mixing and non-parallelism
is necessary)

Antisymmetric spinor

Analogous triplet state in
the 2-band, spin-1/2 case:

$$|T_{\uparrow\uparrow}\rangle = \left|\Psi^A_{1,2}\right\rangle \otimes |1, 1\rangle$$

If we kill the L holes, we kill the minority-symmetry components and the M mixing:

$$
\begin{aligned}
|\mathbb{S}\rangle &\to \sqrt{2}\,\left|\Psi^S_{1H,2H}\right\rangle \otimes \frac{1}{\sqrt{2}}(|0, 0\rangle + |2, 0\rangle), \\
|T_{z,+}\rangle &\to \sqrt{2}\,\left|\Psi^A_{1H,2H}\right\rangle \otimes |3, 3\rangle, \\
|T_{z,0}\rangle &\to \sqrt{2}\,\left|\Psi^A_{1H,2H}\right\rangle \otimes \frac{1}{\sqrt{10}}(3|1, 0\rangle + |3, 0\rangle), \\
|T_{z,-}\rangle &\to \sqrt{2}\,\left|\Psi^A_{1H,2H}\right\rangle \otimes |3, -3\rangle.
\end{aligned}
$$

Comparison of the Hubbard model with the numerical results:

$p_{k,J,M}$ is the weight of the (*J, M*) spinor in state *k*

The model predicts specific relations between several values of $p_{k,J,M}$, independently of the specific orbital wave functions. For example (taken from a triplet state):

$$\ldots + \sqrt{2}\,|\Psi^{A}_{1L,2L}\rangle \otimes \left(\sqrt{\frac{2}{5}}\,|1,-1\rangle + \sqrt{\frac{3}{5}}\,|3,-1\rangle\right)\ldots \quad \text{implies} \quad \frac{p_{2,3,-1}}{p_{2,1,-1}} = \frac{3}{2}$$

There are 18 relations similar to this for the predicted spinor weights in the singlet and triplet.

Comparison with the numerics:

- All relations satisfied within an accuracy of 10^{-4} – 10^{-3}
- Spinors not predicted by the model, total weight: 10^{-3} – 10^{-2}
- Minority-symmetry states: 10^{-2}

Recap (2)

- Single- and two-hole states exhibit a small degree of entanglement, due to either small band mixing, or parallelism of the envelope functions, or both;
- They are superpositions of spinors with different eigenvalues of the angular momentum operators;
- A four-band version of the Hubbard model is able to account for the mixing (qualitatively and quantitatively);
- The source of even/odd J mixing in the two-hole states is due to the presence of distinct heavy- and light-hole envelope functions (i.e., the same source of spin-orbital entanglement);
- Possible extension to large arrays of qubits.

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Interacting holes in Si and Ge double quantum dots: From a multiband approach to an effective-spin picture

Andrea Secchi,[*] Laura Bellentani, Andrea Bertoni, and Filippo Troiani
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Works in progress and future works

- Study of the role of strain in increasing tunneling and exchange;

- Study of qubit readout circuits and quantum capacitance;

- Study of decoherence due to charge impurities and phonons.

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Inter- and intraband Coulomb interactions between holes in silicon nanostructures

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PHYSICAL REVIEW APPLIED **16**, 054034 (2021)

Toward Hole-Spin Qubits in Si *p*-MOSFETs within a Planar CMOS Foundry Technology

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