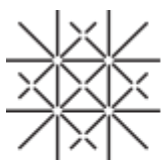


Characterization of the Singlet-Triplet anticrossing in Germanium Nanowire Double Quantum Dots

Jankovic Denis - M1 Internship - 2019

Supervisors : Pr. Dr. Daniel Loss - Dr. Marko Rančić

Condensed Matter Theory and Quantum Computing Group



University
of Basel

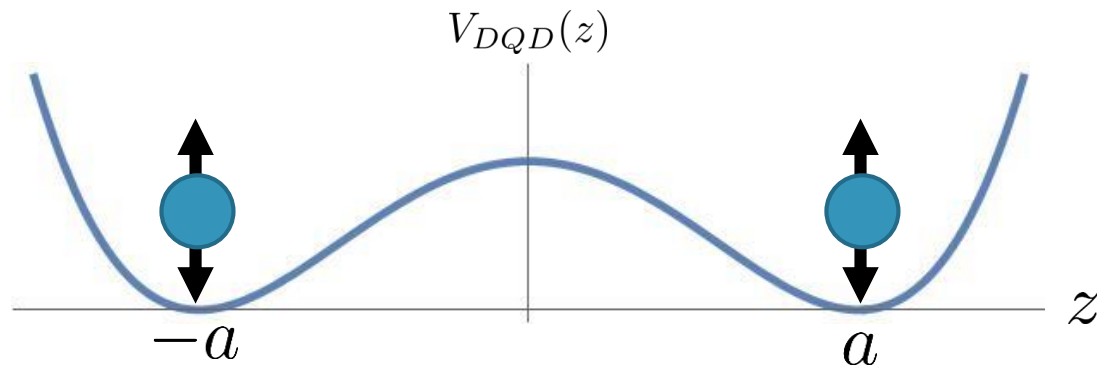
Department of Physics

Double Quantum Dots (DQD)

- ▶ Electron confined by a potential - “Artificial Atom”.
- ▶ Quantum dots (QD) as qubits :
 - ▶ Electronic spin $|\downarrow\rangle = |0\rangle$ $|\uparrow\rangle = |1\rangle$
- ▶ Double quantum dot (DQD) : coupling 2 QD - “Artificial Molecule”
 - ▶ 2 electrons
 - ▶ Possible entanglement
 - ▶ Crucial for universal quantum computers

Our Model - DQD in a Ge Nanowire (Ge NW)

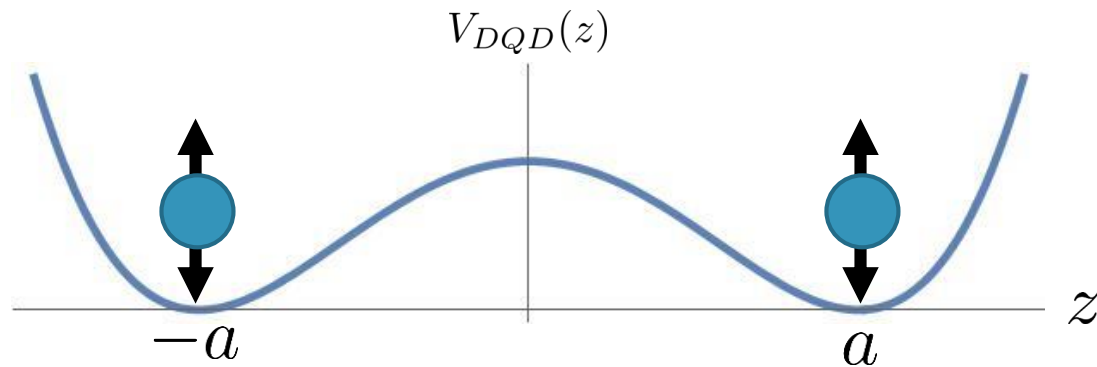
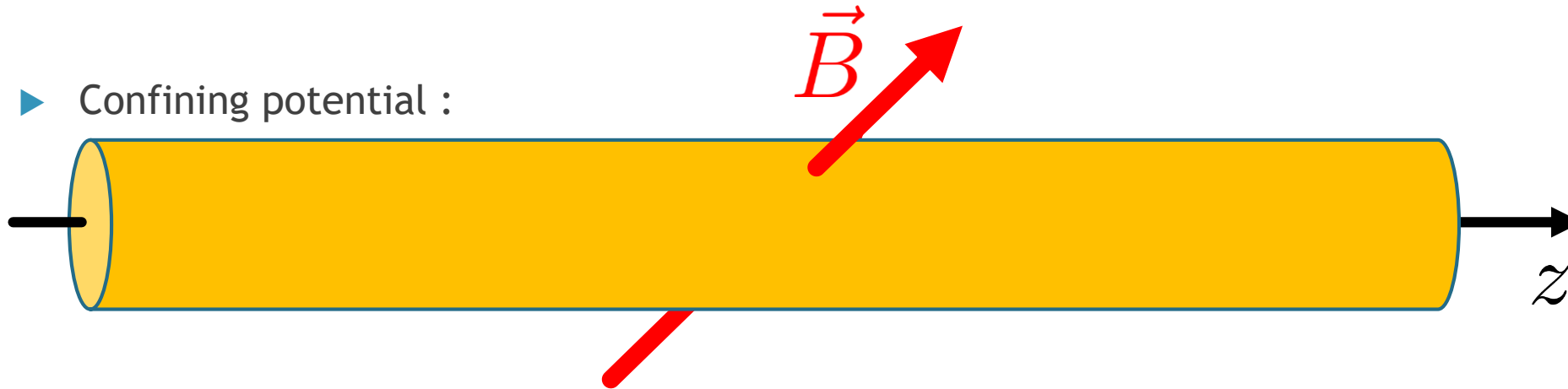
- Confining potential :



$$V_{DQD}(z) = \frac{m\omega_0^2}{2} \left(\frac{1}{4a^2} (z^2 - a^2)^2 \right)$$

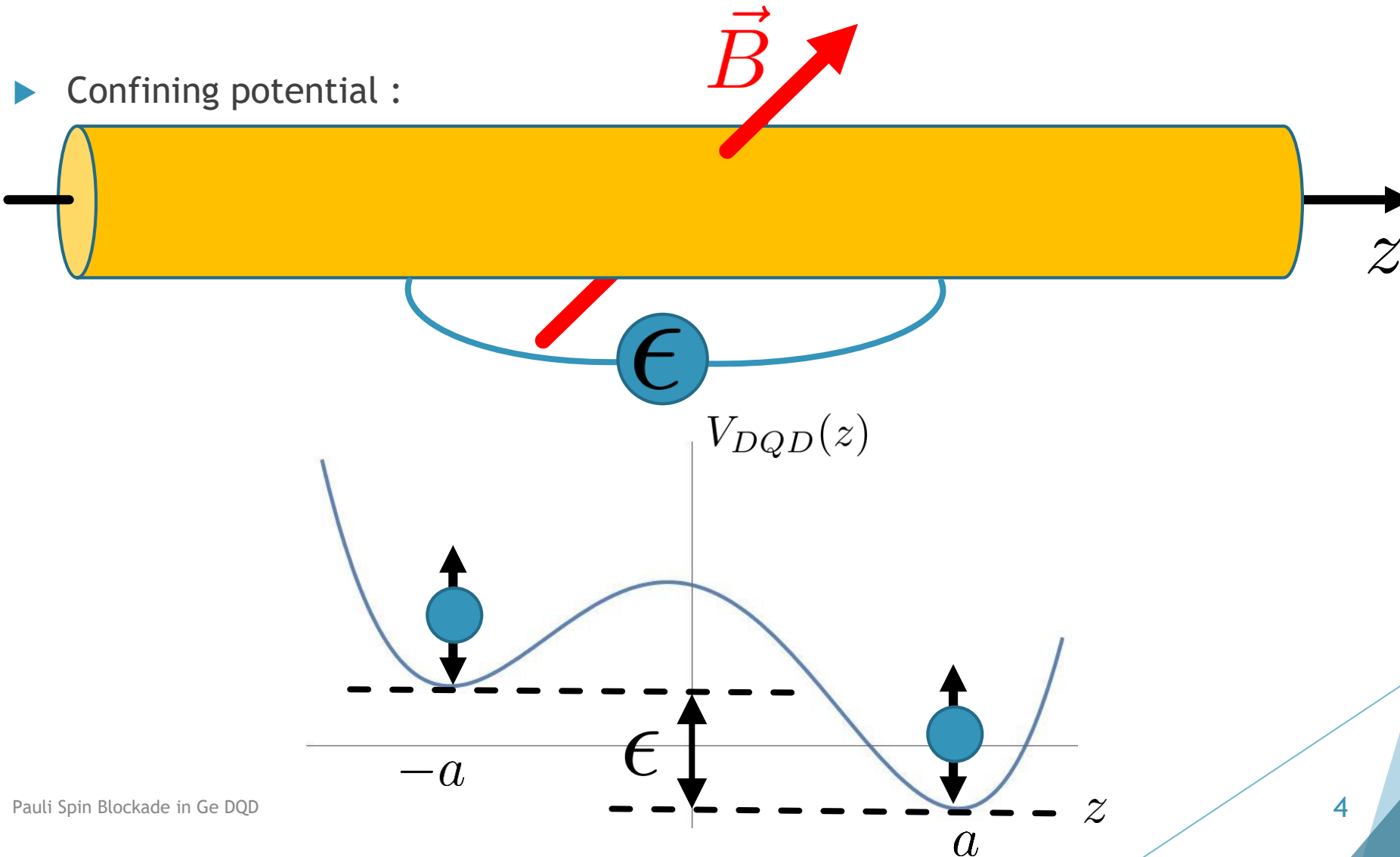
Our Model - DQD in a Ge Nanowire (Ge NW)

- Confining potential :

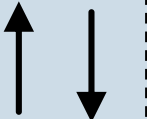

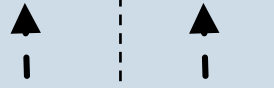

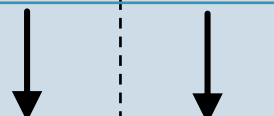
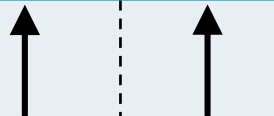


$$V_{DQD}(z) = \frac{m\omega_0^2}{2} \left(\frac{1}{4a^2} (z^2 - a^2)^2 \right)$$

Our Model - DQD in a Ge Nanowire (Ge NW)



Basis States

State	Configuration	S_{tot}
$ (2, 0)S\rangle$		0
$ (0, 2)S\rangle$		
$ (1, 1)S\rangle$		
$ T_0\rangle$		-1
$ T_-\rangle$		
$ T_+\rangle$		
		+1

Model Hamiltonian

$$H = \overbrace{H_{\text{orb}} + H_{\text{Z}} + eV_{\text{bias}}}^{H_0} + H_{\text{SO}}$$

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Model Hamiltonian

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$$H_{\text{orb}} = \sum_{i=1,2} h_i + C$$

Model Hamiltonian

$$H = \overbrace{H_{\text{orb}} + H_Z + eV_{\text{bias}}}^{H_0} + H_{\text{SO}}$$
$$H_{\text{orb}} = \sum_{i=1,2} h_i + C \quad h_i = \frac{\mathbf{p}_i^2}{2m} + V_{DQD}(z_i)$$

Model Hamiltonian

$$H = \overbrace{H_{\text{orb}} + H_Z + eV_{\text{bias}}}^{H_0} + H_{\text{SO}}$$

$$H_{\text{orb}} = \sum_{i=1,2} h_i + C \quad h_i = \frac{\mathbf{p}_i^2}{2m} + V_{DQD}(z_i)$$

$$C = \frac{e^2}{\kappa |z_1 - z_2|}$$

Model Hamiltonian

$$H = \overbrace{H_{\text{orb}} + H_Z + eV_{\text{bias}}}^{H_0} + H_{\text{SO}}$$

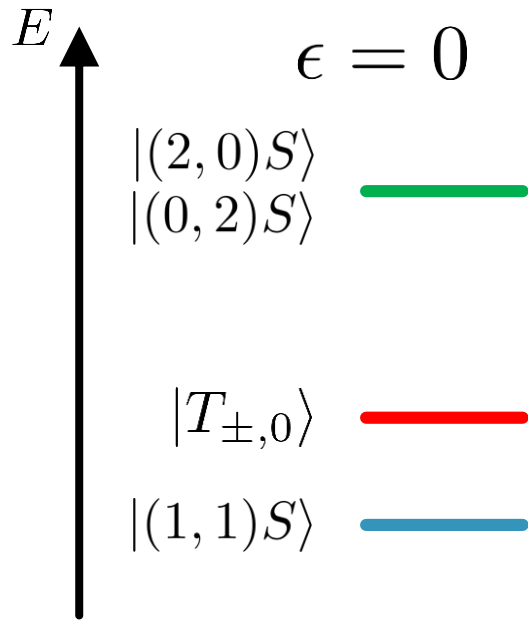
$$H_{\text{orb}} = \sum_{i=1,2} h_i + C \quad h_i = \frac{\mathbf{p}_i^2}{2m} + V_{DQD}(z_i)$$

$$C = \frac{e^2}{\kappa |z_1 - z_2|}$$

$$H_Z = -g\mu_e \vec{B} \cdot \vec{S}_{\text{tot}}$$

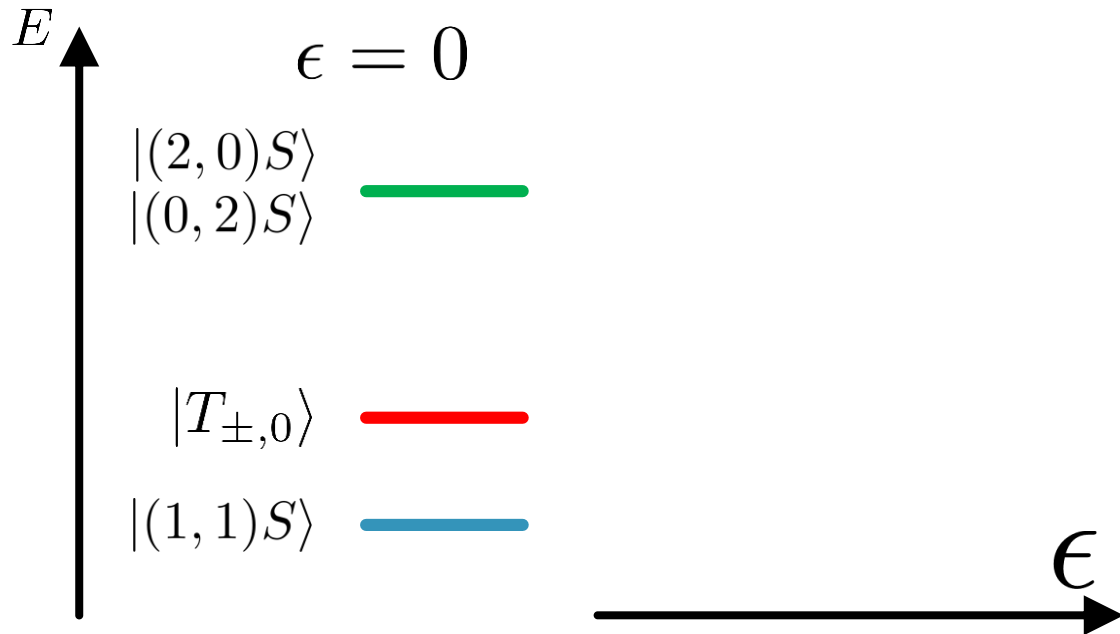
Energy Levels

- ▶ When $B = 0$, depends on detuning ϵ



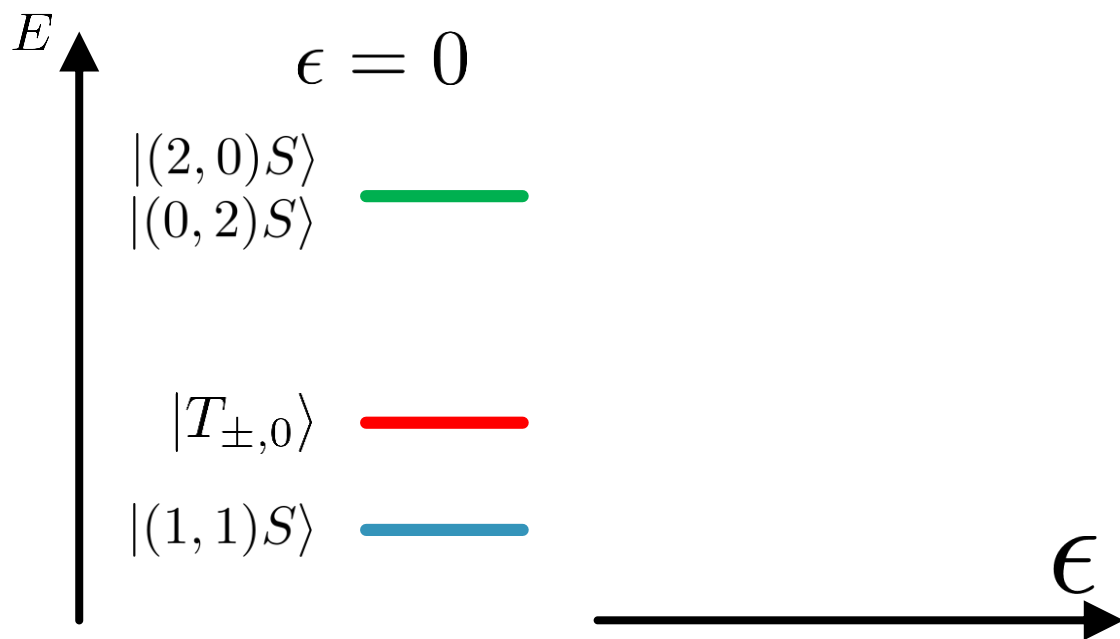
Energy Levels

- ▶ When $B = 0$, depends on detuning ϵ



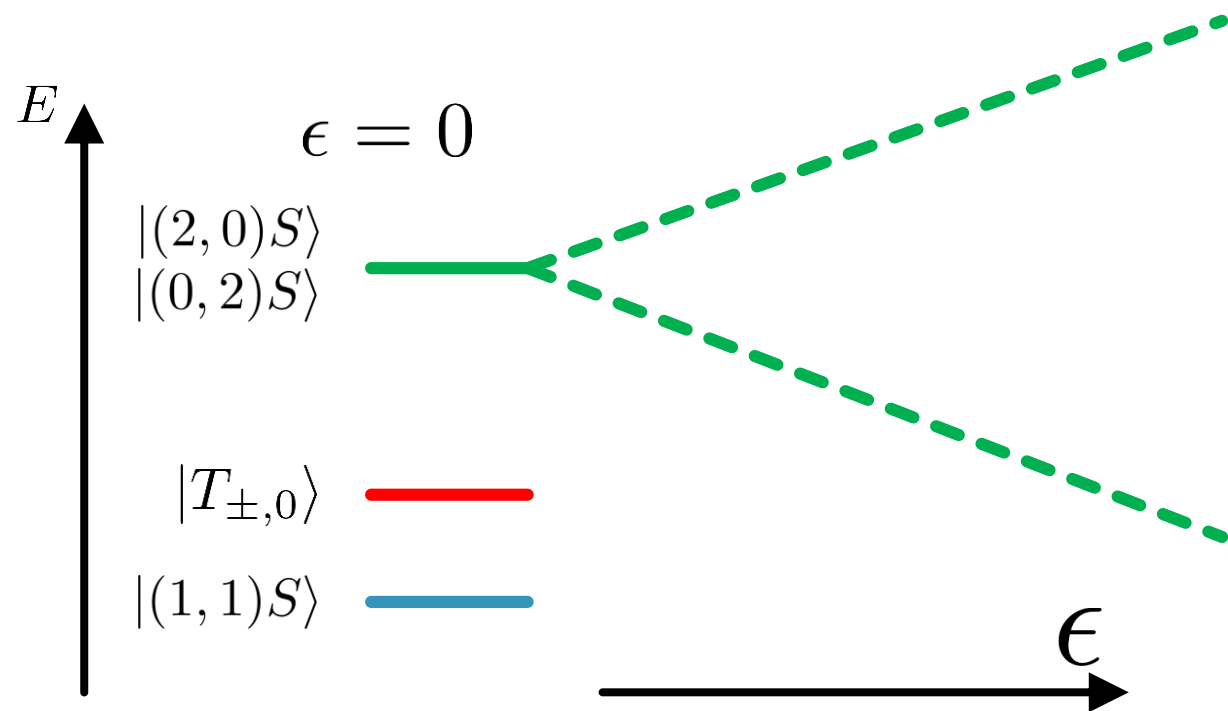
Energy Levels

- ▶ When $B = 0$, depends on detuning ϵ



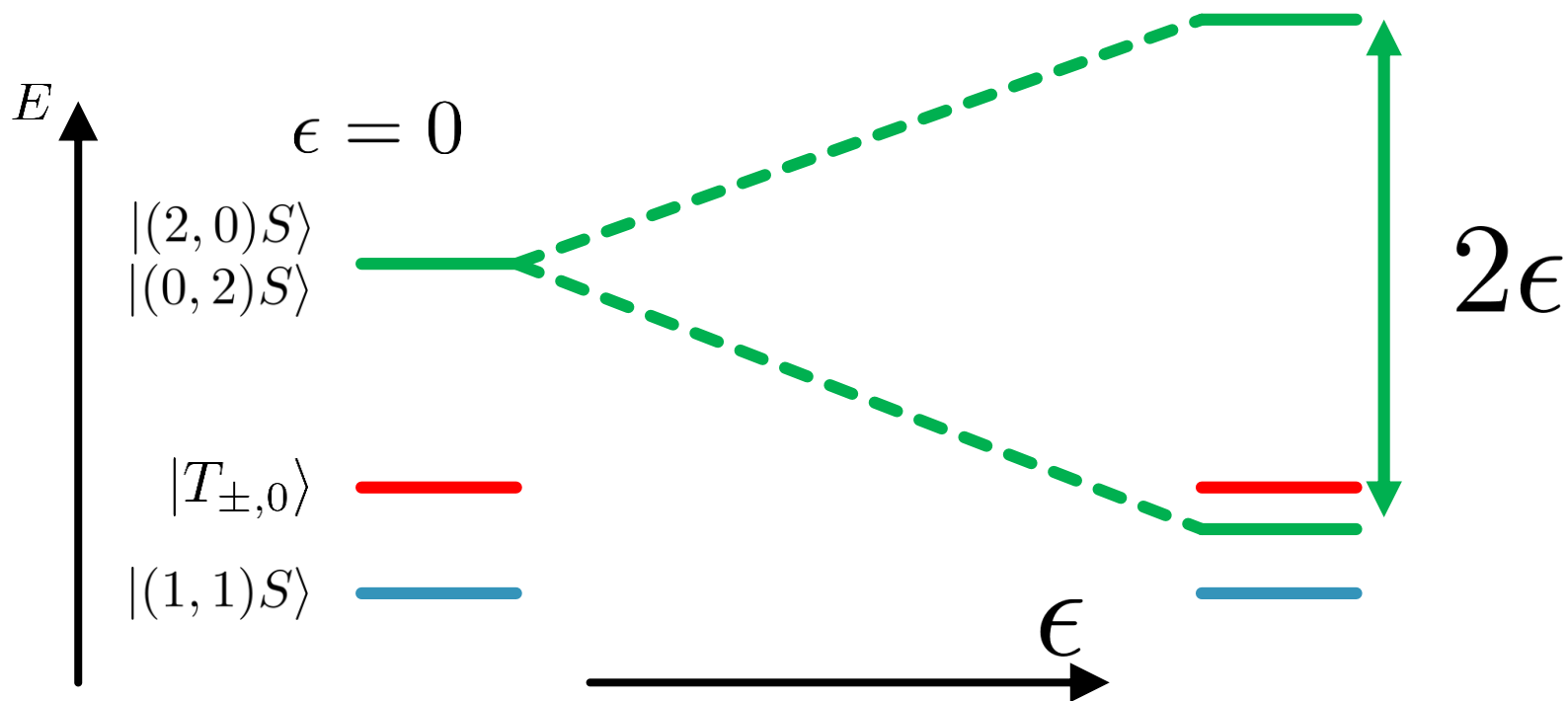
Energy Levels

- ▶ When $B = 0$, depends on detuning ϵ



Energy Levels

- ▶ When $B = 0$, depends on detuning ϵ



Energy Levels

- ▶ $|\epsilon|$ big (comparing to other energies)

$$|S^+\rangle = \sin \psi |(1, 1)S\rangle - \cos \psi |(0, 2)S\rangle$$

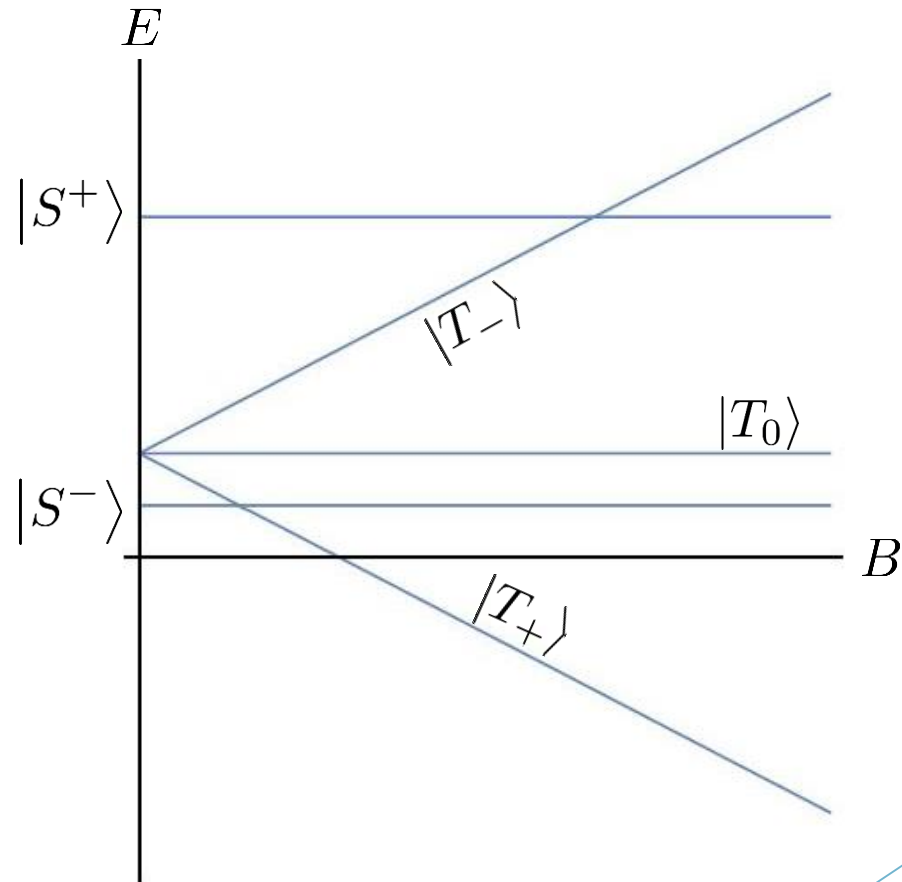
$$|S^-\rangle = \cos \psi |(1, 1)S\rangle + \sin \psi |(0, 2)S\rangle$$

Energy Levels

- ▶ $|\epsilon|$ big (comparing to other energies)

$$|S^+\rangle = \sin \psi |(1, 1)S\rangle - \cos \psi |(0, 2)S\rangle$$

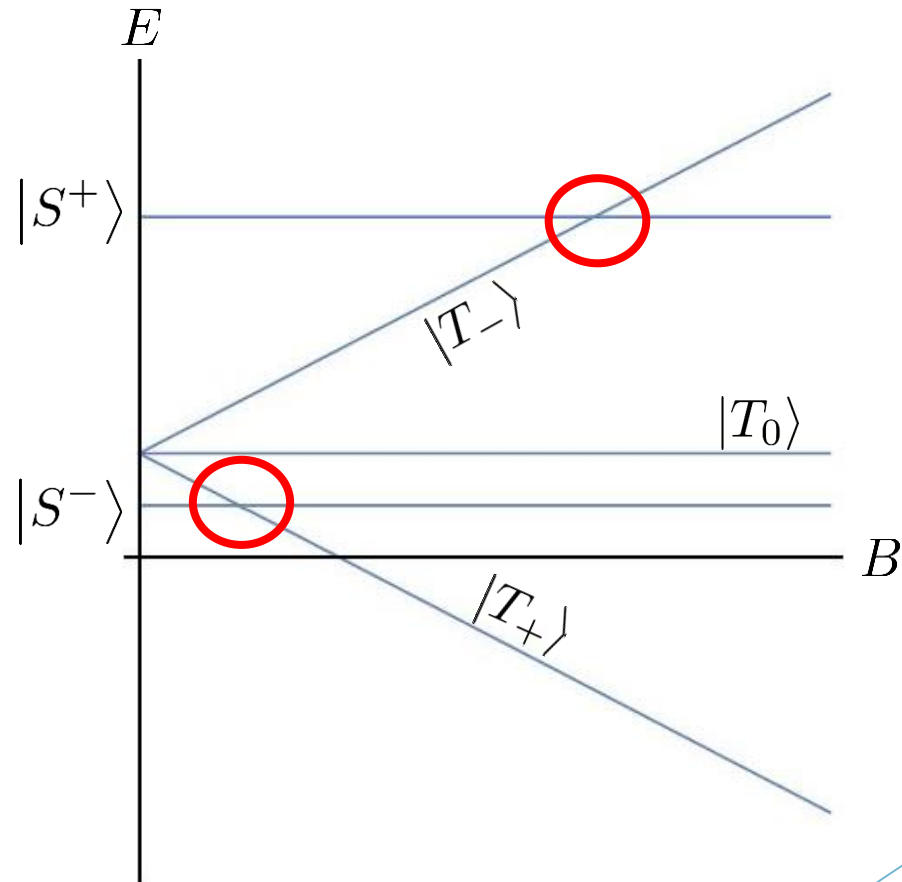
$$|S^-\rangle = \cos \psi |(1, 1)S\rangle + \sin \psi |(0, 2)S\rangle$$



Energy Levels

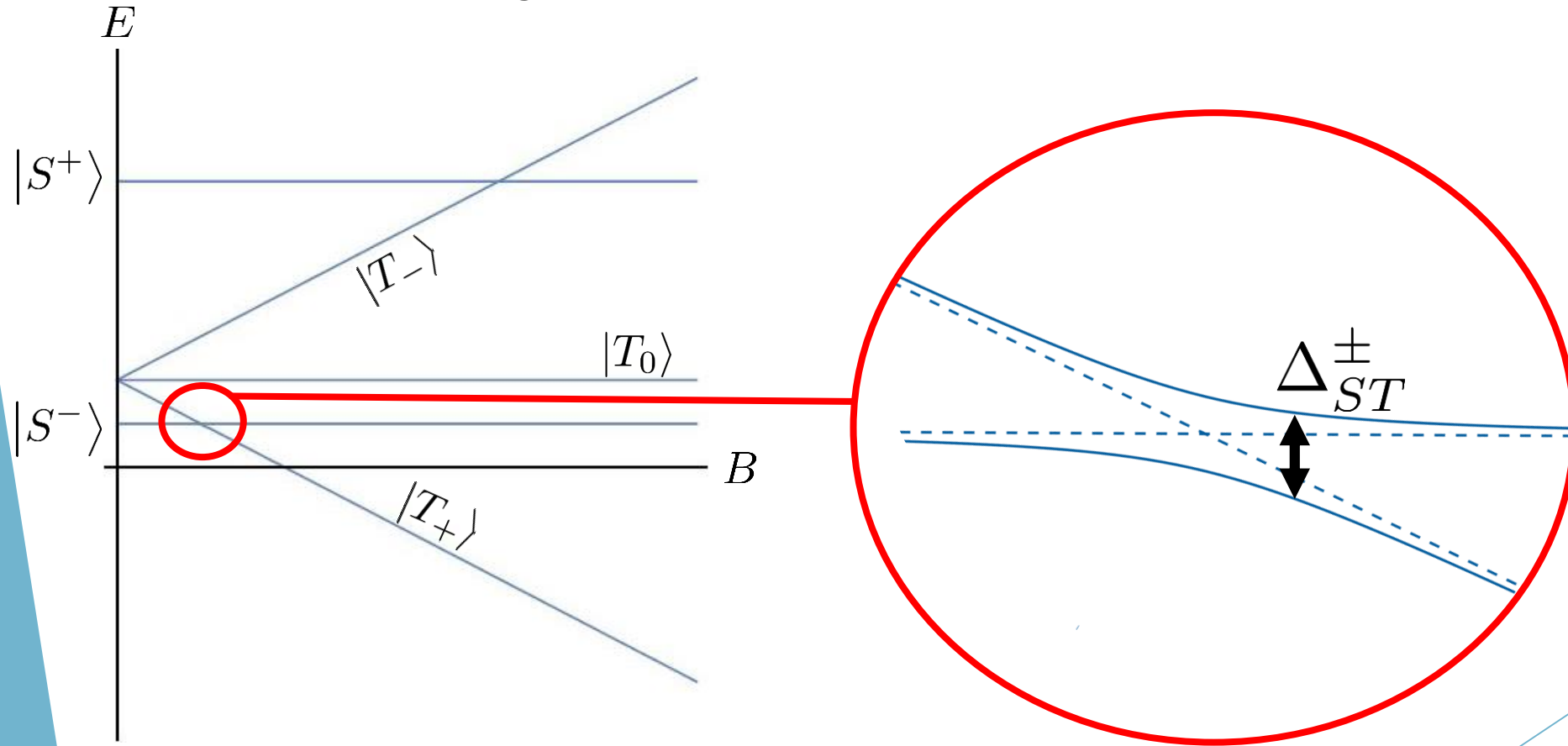
- ▶ $|\epsilon|$ big (comparing to other energies)

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$$|S^-\rangle = \cos \psi |(1, 1)S\rangle + \sin \psi |(0, 2)S\rangle$$



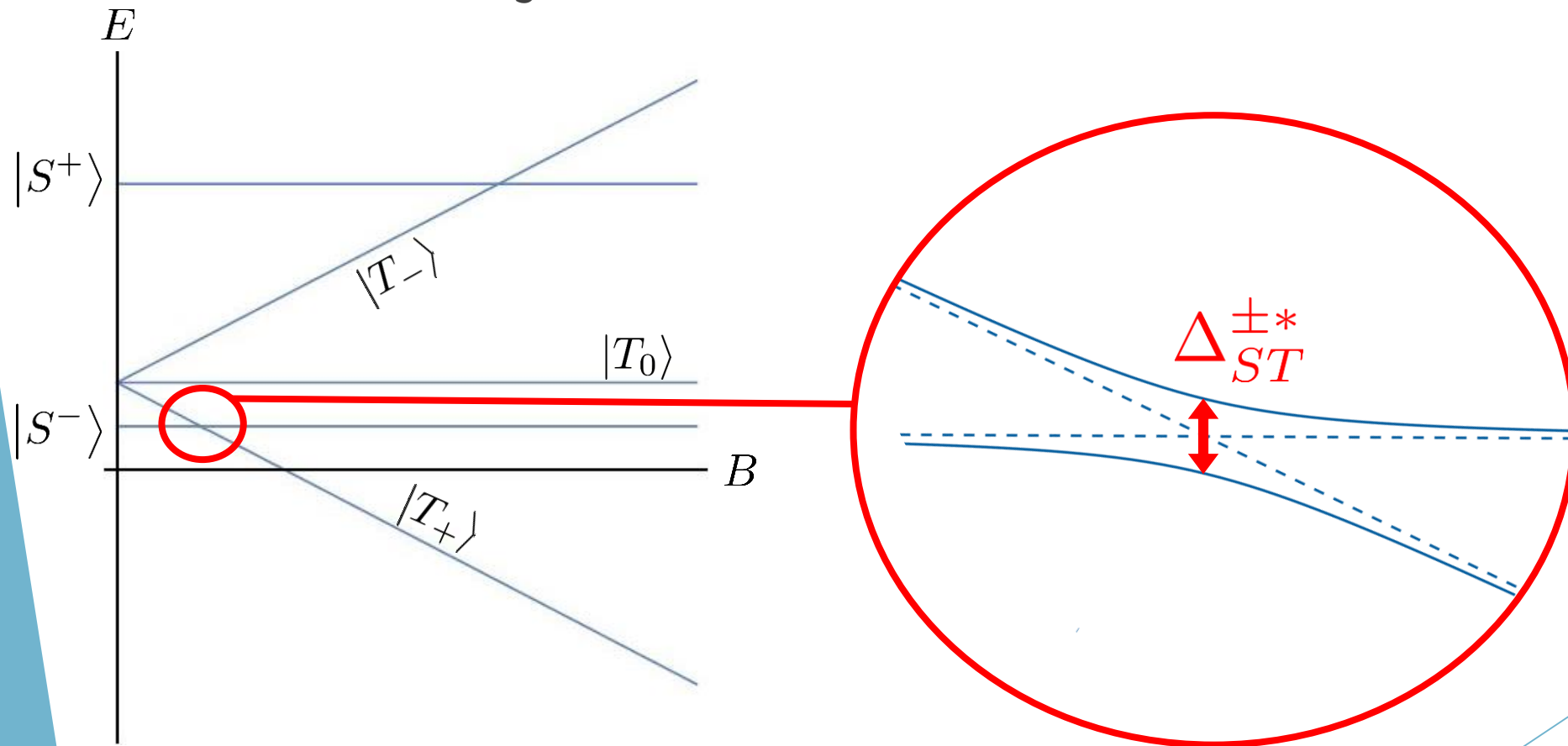
Splitting width minimalization

► At the anticrossing :



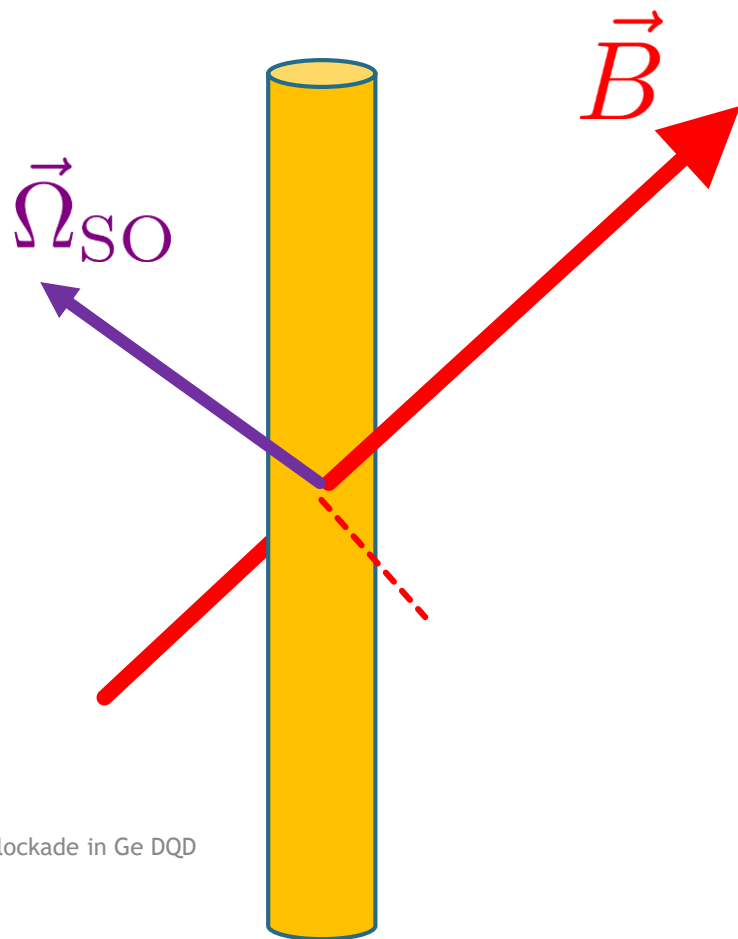
Splitting width minimalization

► At the anticrossing :



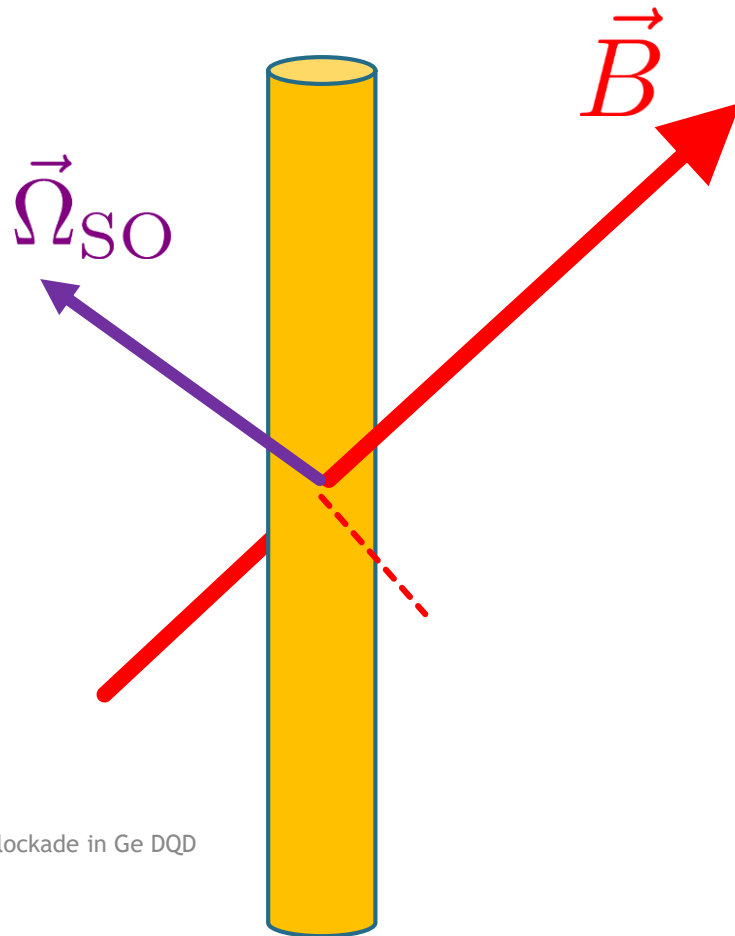
Spin-Orbit Coupling

$$H_{SO} = k_z \vec{\Omega}_{SO} \cdot \underline{\vec{\sigma}}$$



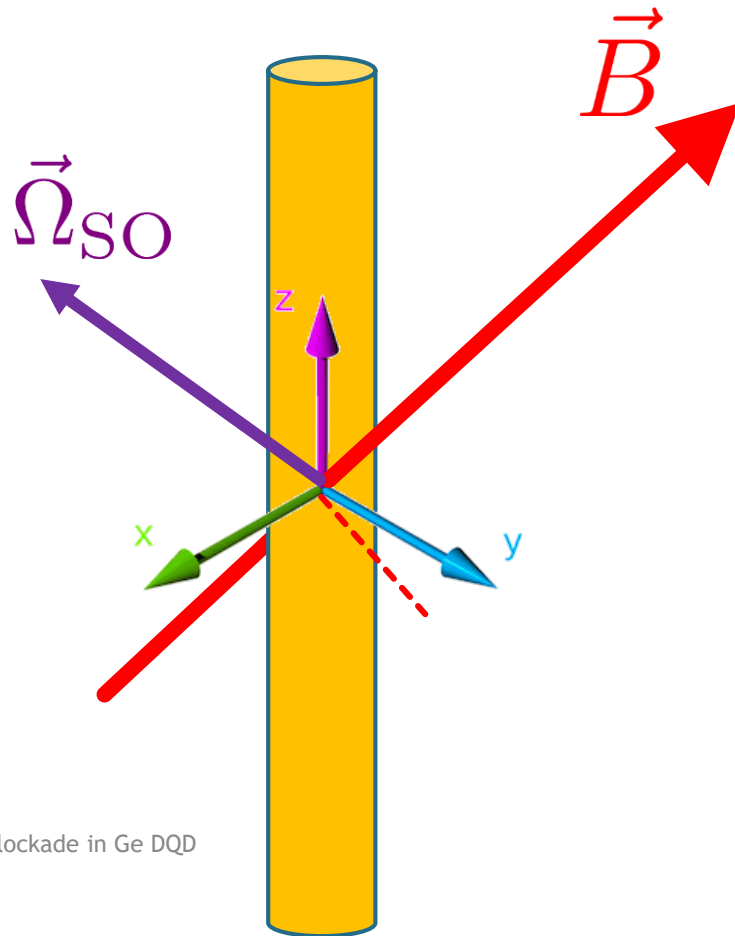
Spin-Orbit Coupling

$$H_{SO} = k_z \vec{\Omega}_{SO} \cdot \vec{\sigma}$$



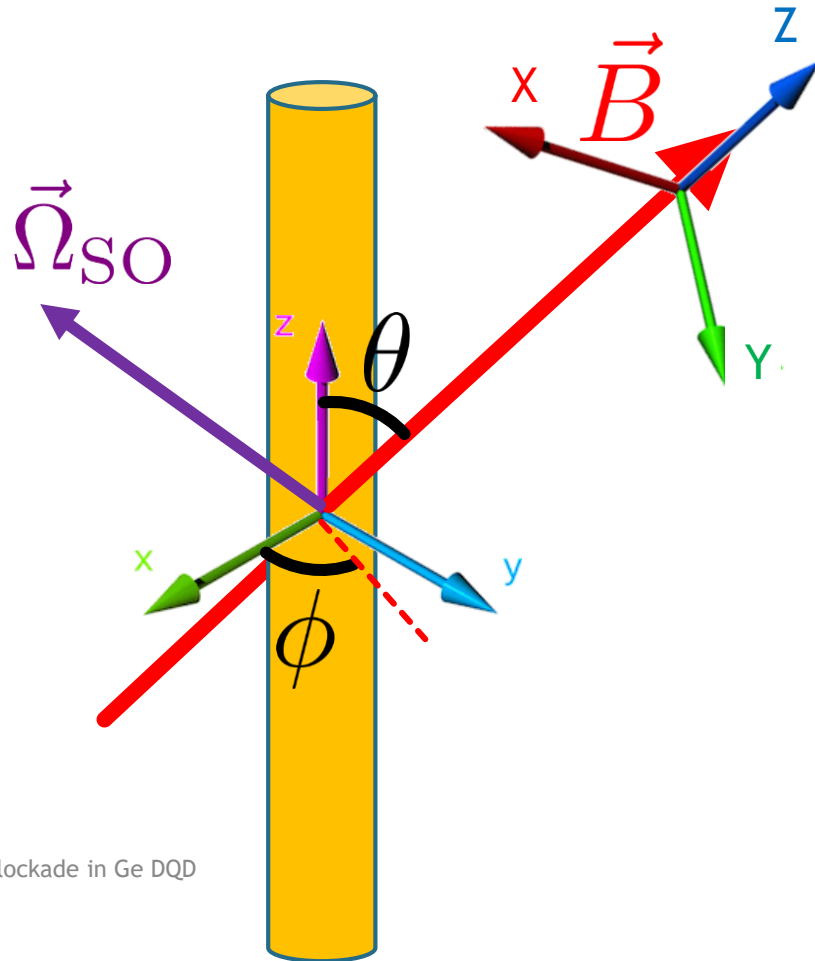
Spin-Orbit Coupling

$$H_{SO} = k_z \vec{\Omega}_{SO} \cdot \vec{\sigma}$$



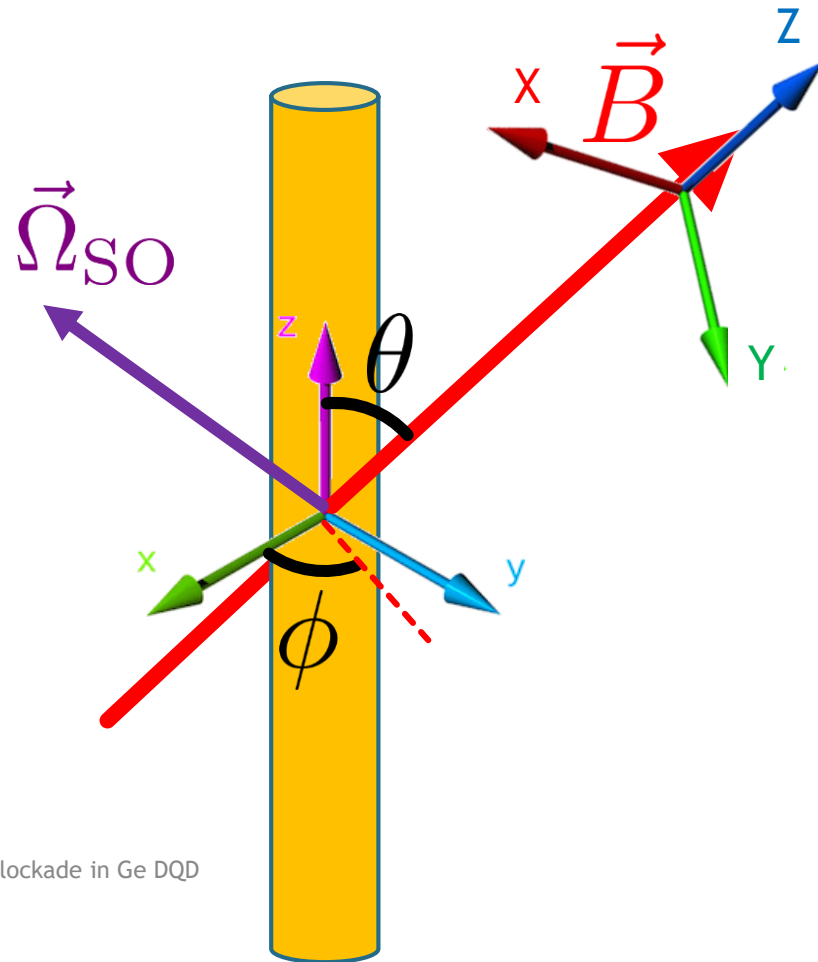
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Spin-Orbit Coupling

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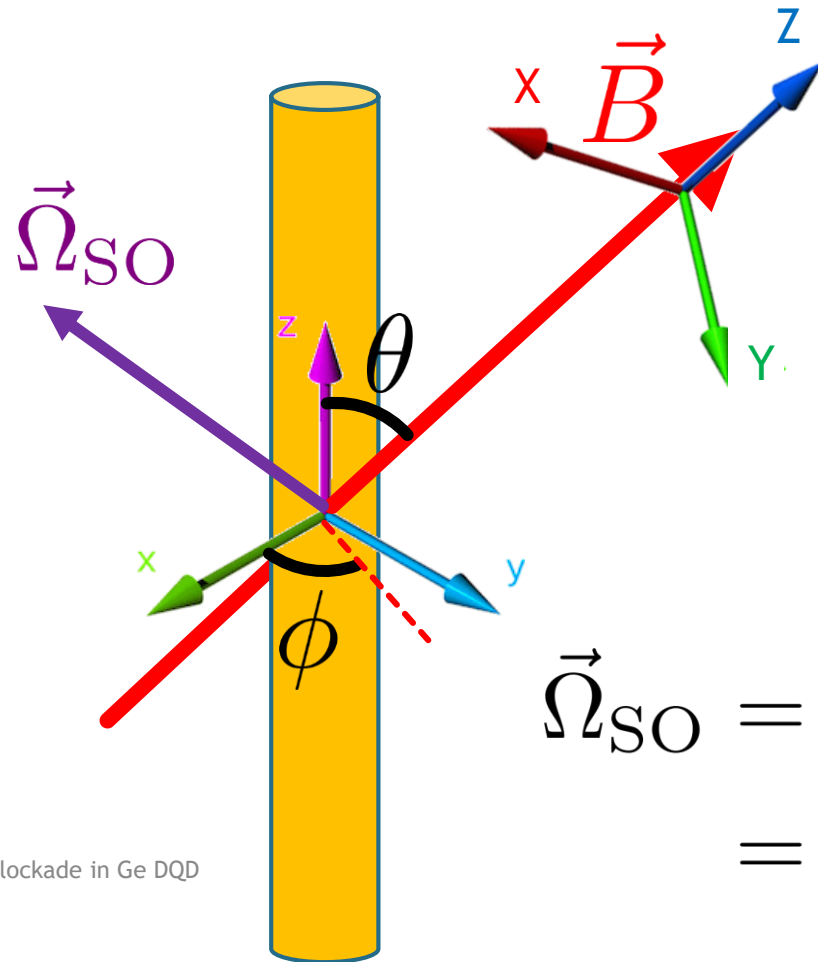
$$\underline{\sigma}_X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\underline{\sigma}_Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\underline{\sigma}_Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Spin-Orbit Coupling

$$H_{SO} = k_z \vec{\Omega}_{SO} \cdot \vec{\sigma}$$



$$\underline{\sigma}_X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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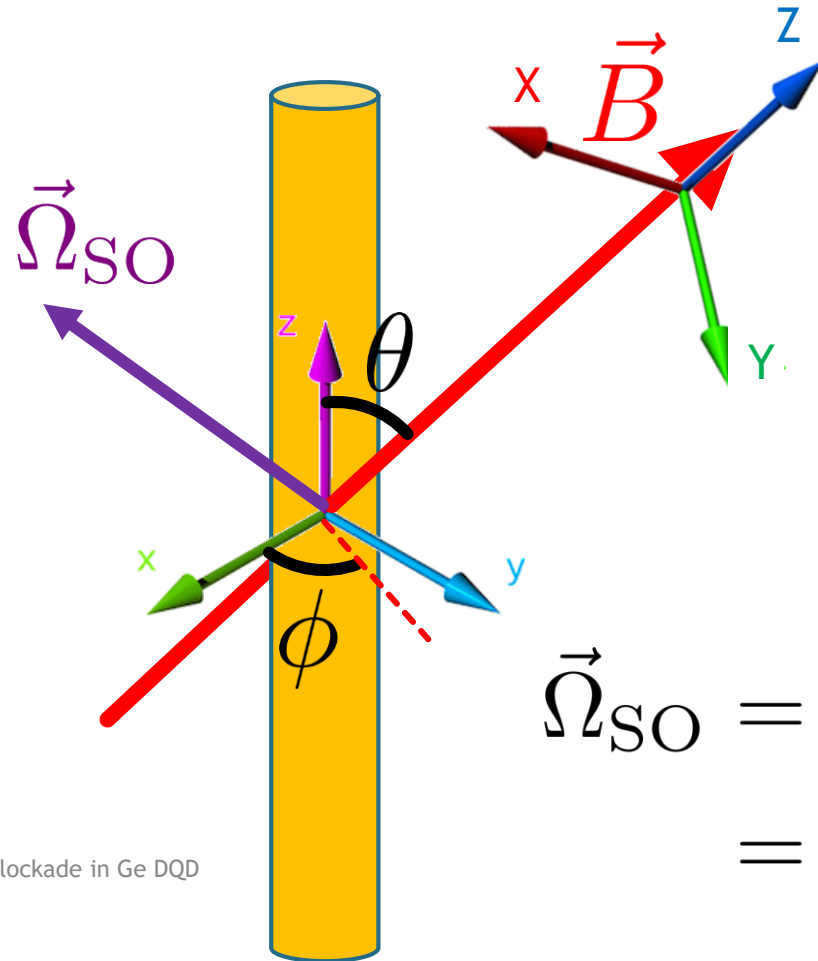
$$\underline{\sigma}_Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\vec{\Omega}_{SO} = (\alpha_X, \alpha_Y, \beta_Z) \vec{B}$$

$$= (\alpha_x, \alpha_y, \beta_z)_{NW}$$

Spin-Orbit Coupling

$$H_{SO} = k_z \vec{\Omega}_{SO} \cdot \vec{\sigma} = \alpha_X k_z \underline{\sigma}_X + \alpha_Y k_z \underline{\sigma}_Y + \beta_Z k_z \underline{\sigma}_Z$$



$$\underline{\sigma}_X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\underline{\sigma}_Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\underline{\sigma}_Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\begin{aligned} \vec{\Omega}_{SO} &= (\alpha_X, \alpha_Y, \beta_Z) \vec{B} \\ &= (\alpha_x, \alpha_y, \beta_z) \text{NW} \end{aligned}$$

Effective Hamiltonian near the anticrossing

► Basis : $\{|S^\pm\rangle, |T_\mp\rangle\}$

$$H_{\text{SO}}^\pm = \langle S^\pm | H_{\text{SO}} | T_\mp \rangle$$

$$H_{\text{cross}}^\pm = \begin{pmatrix} E_{S^\pm} & H_{\text{SO}}^\pm \\ (H_{\text{SO}}^\pm)^* & E_{T_\mp} \end{pmatrix}$$

Anti-crossing width

► Basis : $\{|S^\pm\rangle, |T_\mp\rangle\}$

$$H_{\text{SO}}^\pm = \langle S^\pm | H_{\text{SO}} | T_\mp \rangle$$

$$H_{\text{cross}}^\pm = \begin{pmatrix} E_0 - \frac{\Delta E}{2} & H_{\text{SO}}^\pm \\ (H_{\text{SO}}^\pm)^* & E_0 + \frac{\Delta E}{2} \end{pmatrix}$$

Anti-crossing width

► Basis : $\{|S^\pm\rangle, |T_\mp\rangle\}$

$$H_{\text{SO}}^\pm = \langle S^\pm | H_{\text{SO}} | T_\mp \rangle$$

$$H_{\text{cross}}^\pm = \begin{pmatrix} E_0 - \frac{\Delta E}{2} & H_{\text{SO}}^\pm \\ (H_{\text{SO}}^\pm)^* & E_0 + \frac{\Delta E}{2} \end{pmatrix}$$

$$\Delta_{ST}^{\pm*} = 2|H_{\text{SO}}^\pm|$$

Anti-crossing width

► Basis : $\{|S^\pm\rangle, |T_\mp\rangle\}$

$$H_{\text{SO}}^\pm = \langle S^\pm | H_{\text{SO}} | T_\mp \rangle$$

$$H_{\text{cross}}^\pm = \begin{pmatrix} E_0 - \frac{\Delta E}{2} & H_{\text{SO}}^\pm \\ (H_{\text{SO}}^\pm)^* & E_0 + \frac{\Delta E}{2} \end{pmatrix}$$

$$\langle (0, 2)S | H_{\text{SO}} | T_\pm \rangle = \langle \phi_L | k_z | \phi_R \rangle (\alpha_X + i\alpha_Y)$$

$$\langle (1, 1)S | H_{\text{SO}} | T_{\pm,0} \rangle = 0$$

Anti-crossing width

► Basis : $\{|S^\pm\rangle, |T_\mp\rangle\}$

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$$|S^-\rangle = \cos \psi |(1, 1)S\rangle + \sin \psi |(0, 2)S\rangle$$

Anti-crossing width

► Basis : $\{|S^\pm\rangle, |T_\mp\rangle\}$

$$H_{\text{SO}}^\pm = \langle S^\pm | H_{\text{SO}} | T_\mp \rangle$$

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$$|S^+\rangle = \sin \psi |(1, 1)S\rangle - \cos \psi |(0, 2)S\rangle$$

$$|S^-\rangle = \cos \psi |(1, 1)S\rangle + \sin \psi |(0, 2)S\rangle$$

$$H_{\text{SO}}^+ = -\cos \psi \langle \phi_L | k_z | \phi_R \rangle [(\cos \theta \cos \phi \mp i \sin \phi) \alpha_x + (\cos \theta \sin \phi \pm i \cos \phi) \alpha_y - \beta_z \sin \theta]$$

$$H_{\text{SO}}^- = \sin \psi \langle \phi_L | k_z | \phi_R \rangle [(\cos \theta \cos \phi \mp i \sin \phi) \alpha_x + (\cos \theta \sin \phi \pm i \cos \phi) \alpha_y - \beta_z \sin \theta]$$

Results

- ▶ Splitting width : $\Delta_{ST}^{+*}(\vec{B})$

Results

$$B = 5\text{T} \quad m^* = 0.28m_e$$

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$$B = 5\text{T} \quad m^* = 0.28m_e$$

- Splitting width : $\Delta_{ST}^{+*}(\vec{B})$ $\lambda_x = 1.3 \times 10^{-17}m, \lambda_y = 1.8 \times 10^{-17}m, \lambda_z = 1.2 \times 10^{-17}m$

Results

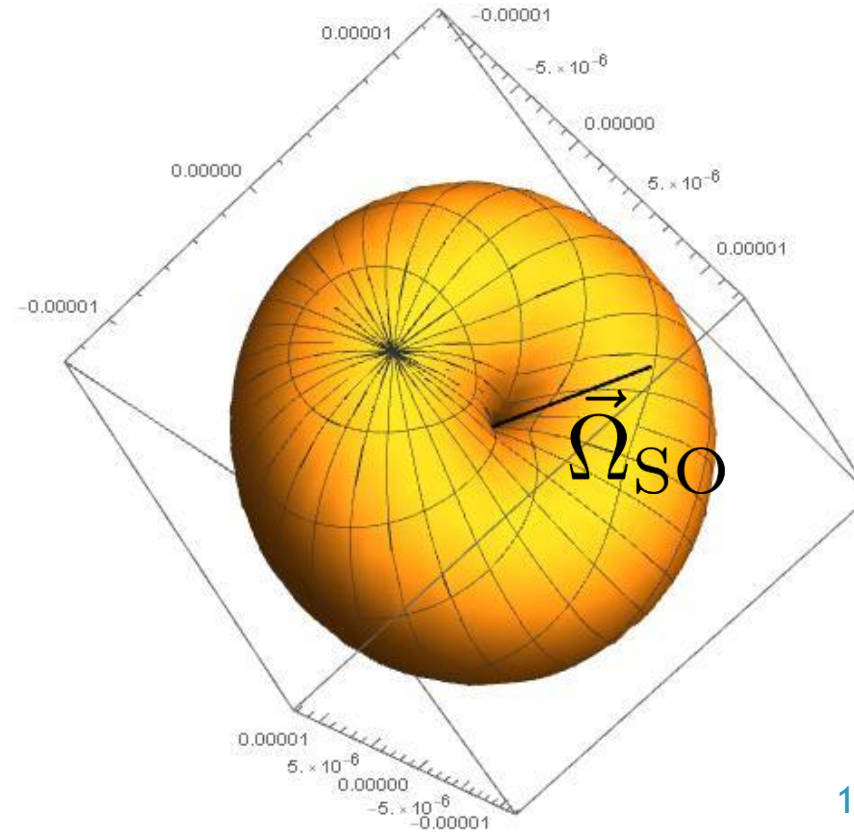
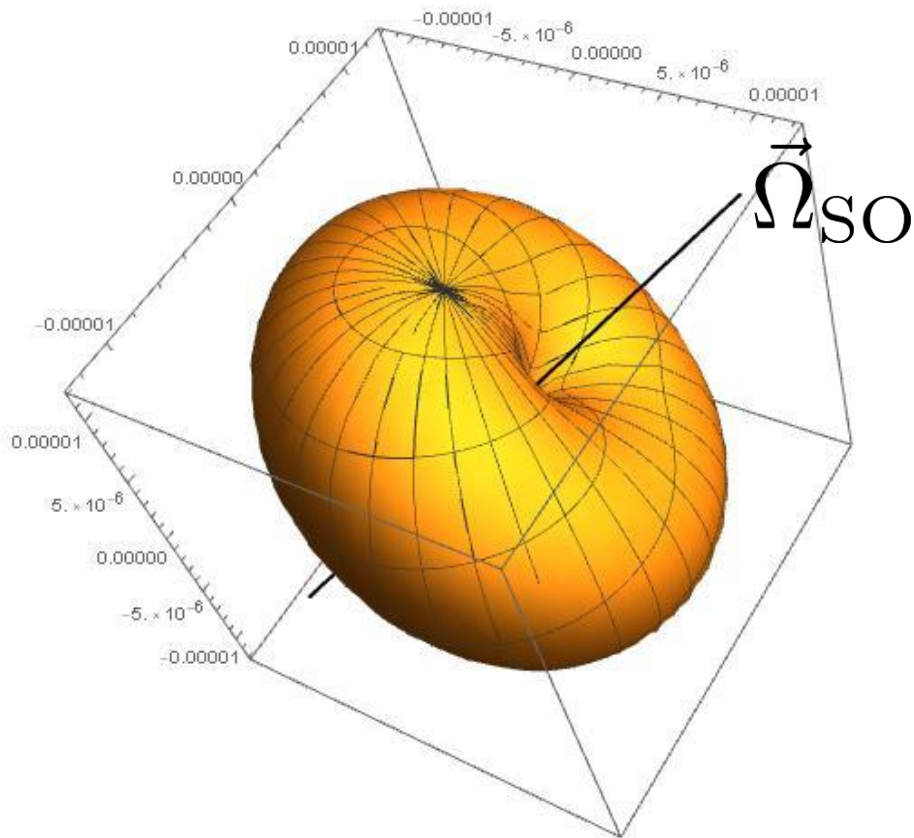
$$\left(\vec{\Omega}_{\text{SO}}\right)_i = \frac{\hbar^2}{m^* \lambda_i} \quad B = 5\text{T} \quad m^* = 0.28m_e$$

► Splitting width : $\Delta_{ST}^{+*}(\vec{B})$ $\lambda_x = 1.3 \times 10^{-17}m, \lambda_y = 1.8 \times 10^{-17}m, \lambda_z = 1.2 \times 10^{-17}m$

Results

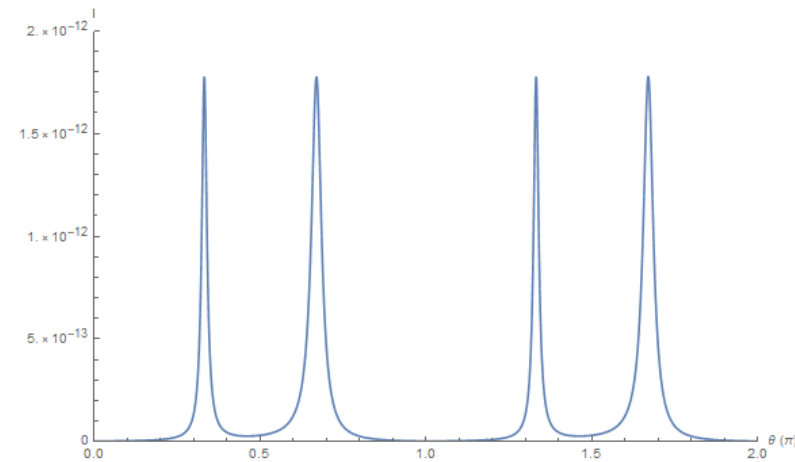
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- Splitting width : $\Delta_{ST}^{+*}(\vec{B})$ $\lambda_x = 1.3 \times 10^{-17}\text{m}, \lambda_y = 1.8 \times 10^{-17}\text{m}, \lambda_z = 1.2 \times 10^{-17}\text{m}$



Further Results & Possible uses

- ▶ Probability of the S-T spin flip (Rabi oscillations)
- ▶ Intensity of the current through NW



- ▶ Spin-flip used in a CNOT double qubit gate
- ▶ S-O coupling is a source of decoherence

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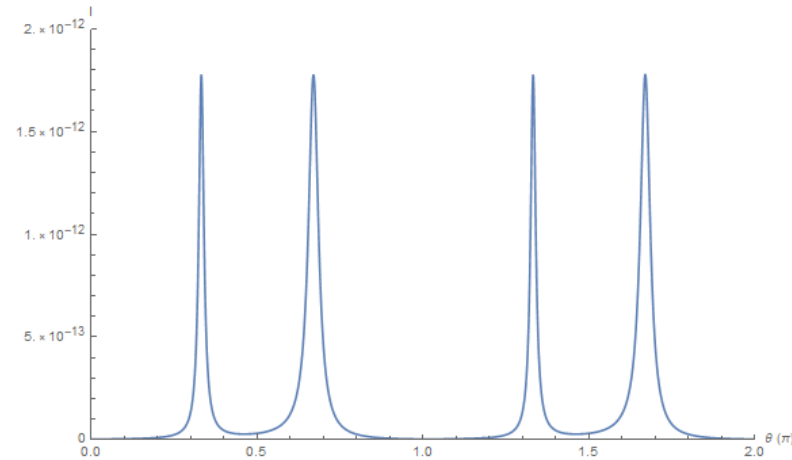
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Thank you !

Questions ?

Further Results & Possible uses

- ▶ Probability of the S-T spin flip (Rabi oscillations)
- ▶ Intensity of the current through NW



- ▶ Spin-flip used in a CNOT double qubit gate
- ▶ S-O coupling is a source of decoherence

Appendix

Quantum Computing

- ▶ Digital bits : 0 or 1
- ▶ Quantum bits (Qubits) : Superposition of $|0\rangle$ and $|1\rangle$

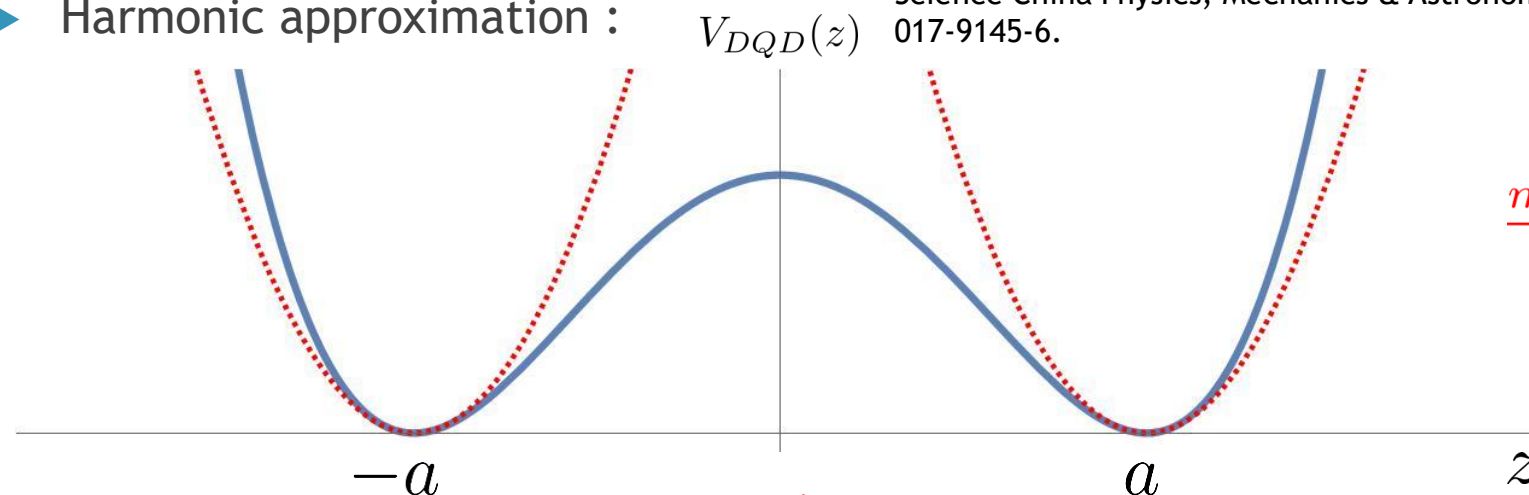
Number of bits	Classical bits	Qubits
1	0 or 1	$c_0 0\rangle + c_1 1\rangle$
2	00, 01, 10 or 11	$c_{00} 00\rangle + c_{01} 01\rangle + c_{10} 10\rangle + c_{11} 11\rangle$
N	1 of 2^N N-uplets	All of the 2^N c_n 's

Molecular Orbit Approximation

Chan & Al. (2018). On the validity of microscopic calculations of double-quantum-dot spin qubits based on Fock-Darwin states.

Science China Physics, Mechanics & Astronomy. 61. 10.1007/s11433-017-9145-6.

► Harmonic approximation :



$$\frac{m\omega_0^2}{2} (z \pm a)^2$$

$$\varphi(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-m\omega x^2/2\hbar}$$

$$\varphi_L(z) = \varphi(z + a)$$

$$\varphi_R(x) = \varphi(z - a)$$

► Hund-Mulliken approach :

$$\Phi_{L,R} = \frac{1}{\sqrt{1 - 2Sg + g^2}} (\varphi_{L,R} - g\varphi_{R,L})$$

Pauli Spin Blockade in Ge DQD

$$S = \int dz \varphi_R^*(z) \varphi_L(z) \quad g = (1 - \sqrt{1 - S^2}) / S$$

Total Wave Functions

State	Configuration	Orbital Part	Spin Part	S_{tot}
$ (2, 0)S\rangle$	$\uparrow \downarrow$	$\Psi_L^d(z_1, z_2) = \Phi_L(z_1)\Phi_L(z_2)$		0
$ (0, 2)S\rangle$	$\uparrow \downarrow$	$\Psi_R^d(z_1, z_2) = \Phi_R(z_1)\Phi_R(z_2)$	$\frac{1}{\sqrt{2}} (\uparrow\downarrow\rangle - \downarrow\uparrow\rangle)$	
$ (1, 1)S\rangle$	$\uparrow \uparrow$	$\Psi_{\pm}^s(z_1, z_2) = \frac{1}{\sqrt{2}} (\Phi_L(z_1)\Phi_R(z_2) \pm \Phi_L(z_2)\Phi_R(z_1))$	$\frac{1}{\sqrt{2}} (\uparrow\downarrow\rangle + \downarrow\uparrow\rangle)$	-1
$ T_0\rangle$	$\downarrow \downarrow$		$ \downarrow\downarrow\rangle$	
$ T_-\rangle$	$\downarrow \uparrow$		$ \uparrow\uparrow\rangle$	
$ T_+\rangle$	$\uparrow \uparrow$			+1

Hamiltonian Matrix

► Basis : $\{|(2, 0)S\rangle, |(0, 2)S\rangle, |(1, 1)S\rangle, |T_+\rangle, |T_0\rangle, |T_-\rangle\}$

$$H_0 = \begin{pmatrix} H_{SS} & 0 \\ 0 & H_{TT} \end{pmatrix}$$

$$H = H_{\text{orb}} + H_Z$$

Hamiltonian Matrix

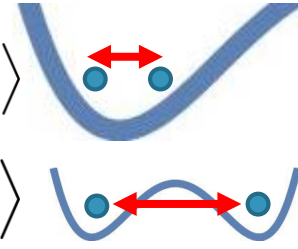
$$H_{\text{orb}} = \sum_{i=1,2} h_i + C$$

► Basis : $\{ |(2,0)S\rangle, |(0,2)S\rangle, |(1,1)S\rangle, |T_+\rangle, |T_0\rangle, |T_-\rangle \}$

$$H_{\text{SS}} = \begin{pmatrix} U + \epsilon & X & -\sqrt{2}t \\ X & U - \epsilon & -\sqrt{2}t \\ -\sqrt{2}t & -\sqrt{2}t & V_+ \end{pmatrix}$$

$$U = \langle \Psi_{\text{L,R}}^d | C | \Psi_{\text{L,R}}^d \rangle$$

$$V_{\pm} = \langle \Psi_{\pm}^s | C | \Psi_{\pm}^s \rangle$$



$$H_{\text{TT}} = \begin{pmatrix} V_- + g\mu_e B & 0 & 0 \\ 0 & V_- & 0 \\ 0 & 0 & V_- - g\mu_e B \end{pmatrix}$$

$$X = \langle \Psi_{\text{L,R}}^d | C | \Psi_{\text{R,L}}^d \rangle$$

$$t = \langle \Phi_{\text{L,R}} | h_{1,2}^0 | \Phi_{\text{R,L}} \rangle - \frac{1}{\sqrt{2}} \langle \Psi_+^s | C | \Psi_{\text{L,R}}^d \rangle$$



Mixing angle

$$U + \epsilon \gg U - \epsilon, V_+ \gg t \gg X$$

$$H_{\text{SS}} = \begin{pmatrix} U + \epsilon & X & -\sqrt{2}t \\ X & U - \epsilon & -\sqrt{2}t \\ -\sqrt{2}t & -\sqrt{2}t & V_+ \end{pmatrix}$$

$$H_{\text{SS}} = \begin{pmatrix} \epsilon & 0 & 0 \\ 0 & U & -\sqrt{2}t \\ 0 & -\sqrt{2}t & V_+ \end{pmatrix}$$

$$\cos 2\psi = \frac{U - V_+}{\sqrt{(U - V_+)^2 + 8t^2}}$$

$$\sin 2\psi = \frac{2\sqrt{2}t}{\sqrt{(U - V_+)^2 + 8t^2}}$$

$$H_{\text{SS}} = \begin{pmatrix} \epsilon & 0 & 0 \\ 0 & E^+ & 0 \\ 0 & 0 & E^- \end{pmatrix}$$

$$|S^+\rangle = \sin \psi |(1, 1)S\rangle - \cos \psi |(0, 2)S\rangle$$

$$|S^-\rangle = \cos \psi |(1, 1)S\rangle + \sin \psi |(0, 2)S\rangle$$

Rabi Oscillation

► Basis : $\{|S^\pm\rangle, |T_\mp\rangle\}$

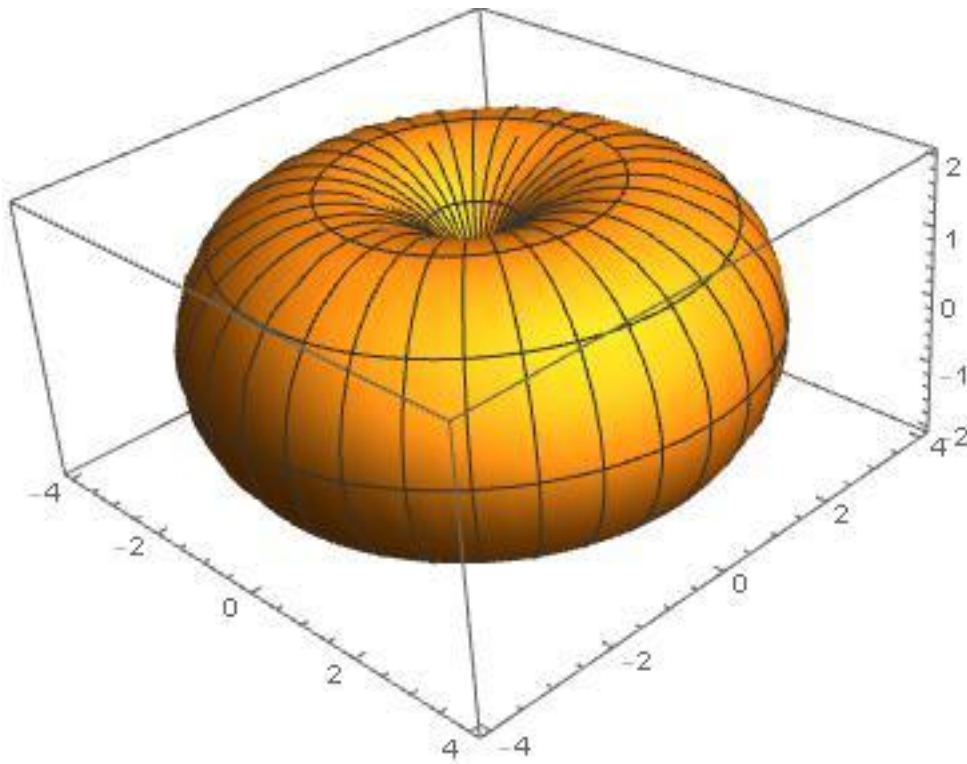
$$H_{\text{SO}}^\pm = \langle S^\pm | H_{\text{SO}} | T_\mp \rangle$$

$$H_{\text{cross}}^\pm = \begin{pmatrix} E_0 - \frac{\Delta E}{2} & H_{\text{SO}}^\pm \\ (H_{\text{SO}}^\pm)^* & E_0 + \frac{\Delta E}{2} \end{pmatrix}$$

$$\Delta E = \pm g(\vec{B})\mu_e B + V_T - V_S$$

g-factor

- Depends on orientation of \vec{B} :



$$g = \vec{\mathcal{G}} \frac{\vec{B}}{B}$$

$$\mathcal{G} = (4, 4, 0.4)$$

Rabi Oscillation

► Basis : $\{|S^\pm\rangle, |T_\mp\rangle\}$

$$H_{\text{SO}}^\pm = \langle S^\pm | H_{\text{SO}} | T_\mp \rangle$$

$$H_{\text{cross}}^\pm = \begin{pmatrix} E_0 - \frac{\Delta E}{2} & H_{\text{SO}}^\pm \\ (H_{\text{SO}}^\pm)^* & E_0 + \frac{\Delta E}{2} \end{pmatrix}$$

$$\Delta E = \pm g(\vec{B})\mu_e B + V_T - V_S \quad \Delta_{ST}^{\pm*} = 2|H_{\text{SO}}^\pm|$$

Rabi Oscillation

► Basis : $\{|S^\pm\rangle, |T_\mp\rangle\}$

$$H_{\text{SO}}^\pm = \langle S^\pm | H_{\text{SO}} | T_\mp \rangle$$

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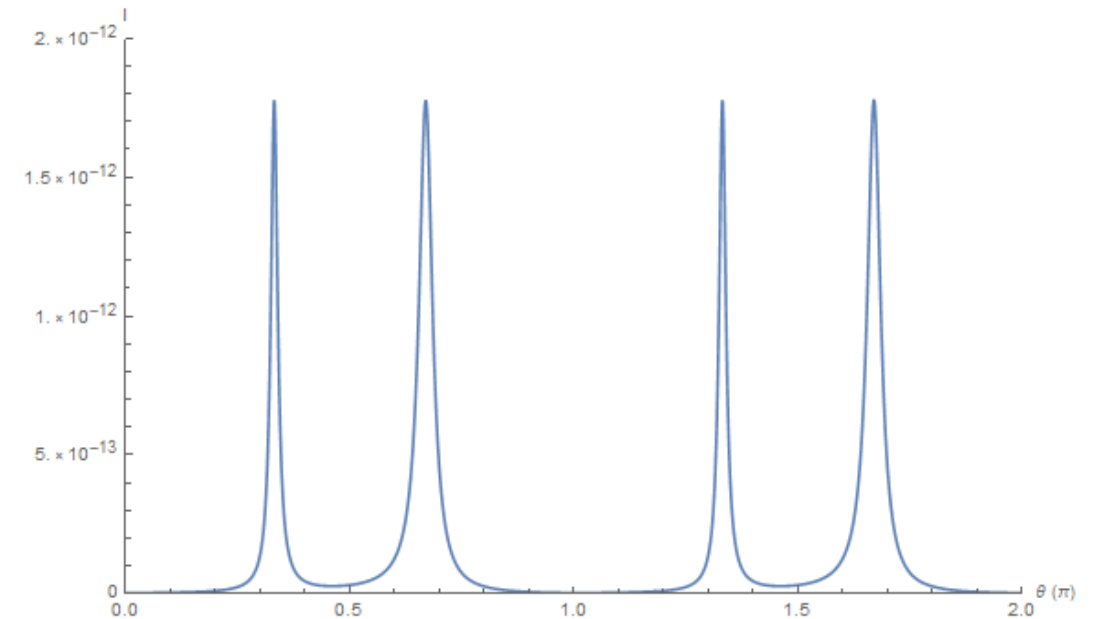
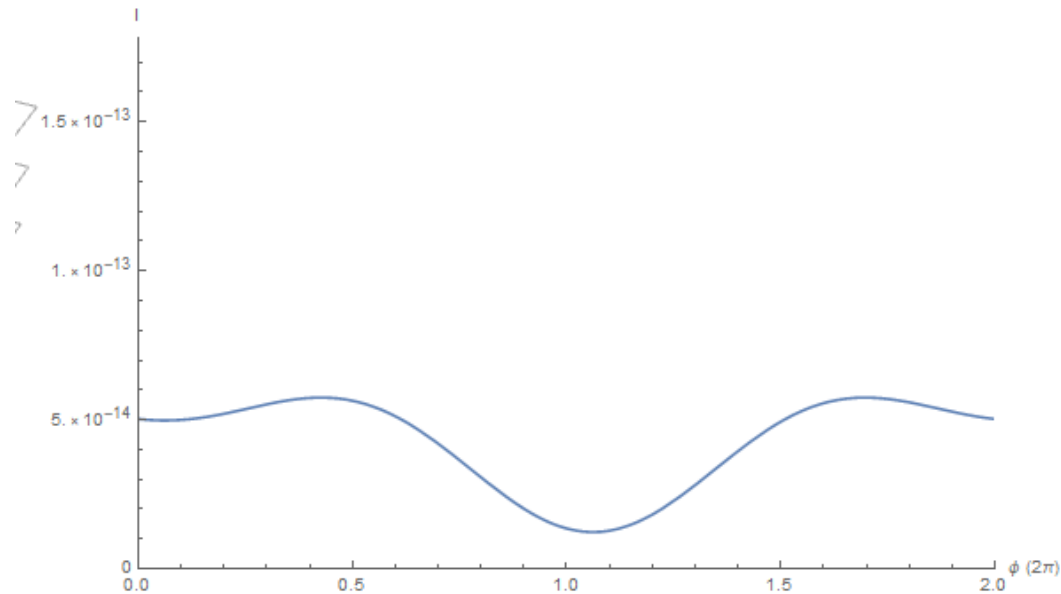
$$\Delta E = \pm g(\vec{B})\mu_e B + V_T - V_S \quad \Delta_{ST}^{\pm*} = 2|H_{\text{SO}}^\pm|$$

$$A_{\text{Rabi}}^\pm = |P_{S^\pm \rightarrow T_\mp}|_{\text{max}} = \frac{(\Delta_{ST}^{\pm*})^2}{(\Delta_{ST}^{\pm*})^2 + \Delta E^2}$$

Results

► Intensity:

$$\lambda_x = 5 \times 10^{-18} m, \lambda_y = 2.5 \times 10^{-17} m, \lambda_z = 1.3 \times 10^{-17} m$$



$$\frac{\Gamma e \Delta_{ST}(\alpha x, \alpha y, \beta, \theta, \phi)^2}{3 \Delta_{ST}(\alpha x, \alpha y, \beta, \theta, \phi)^2 + \Delta E(gx, gy, gz, \theta, \phi)^2 + \left(\frac{\Gamma \hbar b}{2}\right)^2}$$

Two-level system

► Basis : $\{|S^\pm\rangle, |T_\mp\rangle\}$

$$H_{\text{SO}}^\pm = \langle S^\pm | H_{\text{SO}} | T_\mp \rangle$$

$$H_{\text{cross}}^\pm = \begin{pmatrix} E_0 - W & H_{\text{SO}}^\pm \\ (H_{\text{SO}}^\pm)^* & E_0 + W \end{pmatrix}$$

$$W = \frac{E_{T_\mp} - E_{S^\pm}}{2} = \frac{1}{2}(\pm g\mu_e B + V_T - V_S) = \frac{\Delta E}{2}$$

$$\Delta_{ST}^\pm(\vec{B}) = 2\sqrt{|H_{\text{SO}}^\pm(\vec{B})|^2 + \Delta E(\vec{B})^2}$$

$$A_{\text{Rabi}}^\pm = |P_{S^\pm \rightarrow T_\mp}| = \frac{(\Delta_{ST}^{\pm*})^2}{(\Delta_{ST}^\pm)^2}$$