

# Notes on: FAQUAD in Quantum Dots

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## 1 Model

The system that we study is a quantum dot (QD) array populated with heavy holes in presence of a external magnetic field perpendicular to the dots. In absence of spin-orbit coupling (SOC) we can write the second quantization Hamiltonian as

$$H = \sum_{i\sigma} \varepsilon_{i\sigma} n_{i\sigma} + u \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_{i \neq j} \sum_{\sigma} \tau_{ij} \left( c_{i\sigma}^\dagger c_{j\sigma} + H.c. \right), \quad (1)$$

where  $\varepsilon_{i\sigma}$  denoted the energy of the single-particle located in the dot  $i$  with spin  $\sigma = \uparrow, \downarrow = \pm 1/2$ . This energy takes into account the bias energy level of the dot and the Zeeman splitting

$$\varepsilon_{i\sigma} = \varepsilon_i + g\mu_B B\sigma \equiv \varepsilon_i + E_Z\sigma. \quad (2)$$

A typical value of the effective  $g$ -factor for heavy holes in GaAs could be  $g = 1.35$ . The intradot Coulomb interaction  $u$  exist when various particles occupy the same dot. There is also a spin-conserving tunnelling term  $\tau$  between adjacent QD's. Finally, the operator  $c_{i\sigma}$  ( $c_{i\sigma}^\dagger$ ) represents the annihilation (creation) of a hole in the dot  $i$  with spin  $\sigma$ .

## 2 Double Quantum Dot

The energy spectrum for a double quantum dot array (DQD) populated with two heavy holes is given in Fig 1, where we have normalized the instant eigenenergies with the Zeeman splitting energy. It's usual to work with an antisymmetric bias gate for each dot where  $\varepsilon_R = -\varepsilon_L$ , and define the difference as the detuning  $\varepsilon \equiv \varepsilon_R - \varepsilon_L$ . To obtain this results we have excluded one of the double occupation states  $|S(2,0)\rangle$ , which is motivated by the current experiments.

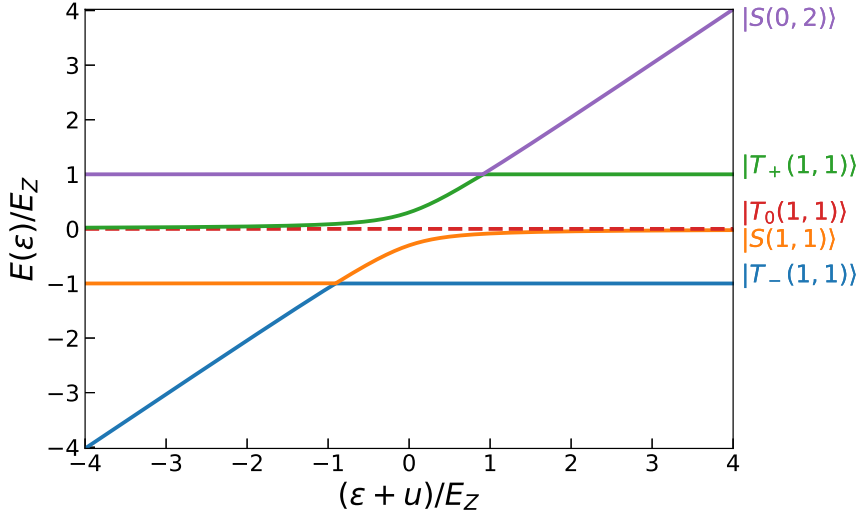


Figure 1: Energy spectrum for the system of a double quantum dot array populated with two heavy holes without spin orbit coupling. The parameters used are  $B = 0.015$  T,  $E_Z = 1.17$   $\mu\text{eV}$ ,  $\tau = 0.25$   $\mu\text{eV}$  and  $u = 2$  meV.

We are only interested in the subspace formed by the two singlets states  $|S(1, 1)\rangle$ ,  $|S(0, 2)\rangle$ , and the **least** energetic triplet estate  $|T_-(1, 1)\rangle$ . With this the Hamiltonian can be easily written with the matrix

$$H = \begin{pmatrix} |T_-(1, 1)\rangle & |S(1, 1)\rangle & |S(0, 2)\rangle \\ -E_Z & 0 & 0 \\ 0 & 0 & \sqrt{2}\tau \\ 0 & \sqrt{2}\tau & \varepsilon + u \end{pmatrix}. \quad (3)$$

In order to couple the singlets and the triplet we can introduce two new terms, the Dresselhaus SOC and the Rashba SOC

$$\begin{aligned} H_D &= \beta(\sigma_+ p_- - m_+ p_- - \sigma_- p_+ p_- p_+) \\ H_R &= i\alpha E_\perp (\sigma_+ p_-^3 - \sigma_- p_+^3). \end{aligned} \quad (4)$$

To keep the computations as much simpler **as** possible we take both SOC parameters to be equal  $\beta = \alpha E_\perp$ . The two new coupling are defined as

$$\begin{aligned} \lambda_1 &= \langle T_-(1, 1) | H_D + H_S | S(1, 1) \rangle \\ \lambda_2 &= \langle T_-(1, 1) | H_D + H_S | S(0, 2) \rangle. \end{aligned} \quad (5)$$

To obtain an analytical expression for this two term **we** can impose the single hole orbital functions with Gaussian shapes **centred** at each dot

$$\psi_i = \frac{1}{l} \sqrt{\frac{2}{\pi}} \exp\left(-\frac{(x - x_i)^2 + y^2}{l^2}\right), \quad (6)$$

where the dot lies in the  $x$  axis,  $d$  is the interdot distance  $x_1 = -x_2 = d/2$ , and  $l$  is the extent of the wave function. After integration we obtain the expressions

$$\begin{aligned} \lambda_1 &= \frac{8\alpha E_\perp d}{l^4} \exp(-d^2/l^2) \\ \lambda_2 &= \frac{4\sqrt{2}\alpha E_\perp d}{l^4} \exp(-d^2/2l^2). \end{aligned} \quad (7)$$

Choosing  $l = d/3$  we observe that  $\lambda_1/\lambda_2 \approx 1/100$ , being the coupling with the double occupation singlet states stronger. An analytical solution for the instant eigenstates is too complex, but we can solve it numerically, obtaining the energy spectrum shown in Fig 2. Our task is to pass from  $|T_-(1,1)\rangle$  to  $S(1,1)$  with the minimum possible

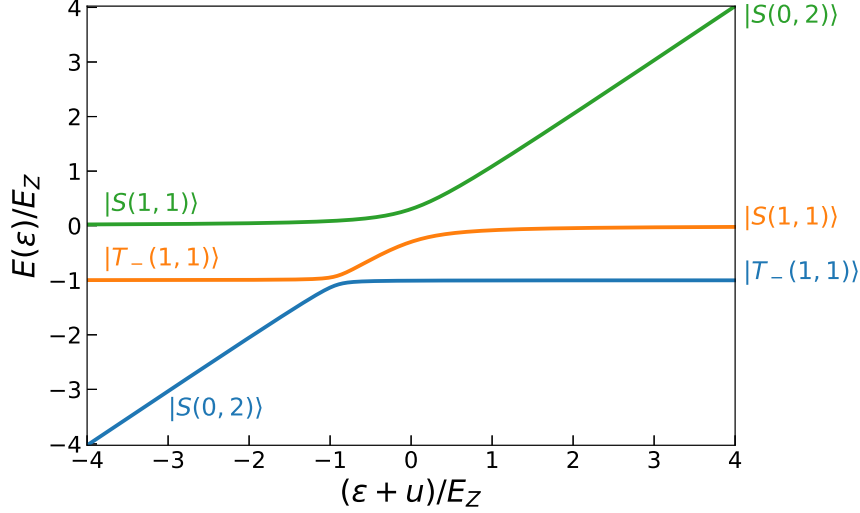


Figure 2: Three lowest energies for the system of a double quantum dot array populated with two heavy holes in presence spin orbit coupling. The parameters used are  $B = 0.015$  T,  $E_Z = 1.17$  meV,  $\tau = 0.25$   $\mu$ eV,  $\lambda_1 = 0.001$   $\mu$ eV,  $\lambda_2 = 0.1$   $\mu$ eV and  $u = 2$  meV.

occupation of  $S(0,2)$ . We have not include any term in the Hamiltonian that flip the spin of the hole without “jumping” to some other qubit, so the only possible transition allowed is

$$|\downarrow, \downarrow\rangle \rightarrow |0, \uparrow\downarrow\rangle \rightarrow \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) . \quad (8)$$

There exist some quasi adiabatic techniques that take advantage of the existence of a dark-state which has no weight in the intermediate step. To check if this is also the case for our system we can compute numerically the instant eigenvectors and extracting the probability to occupy the double occupation singlet state Fig 3. Here we have plotted the value  $|\langle\psi_2|S(0,2)\rangle|^2$  where  $|\psi_2\rangle$  correspond to the state in which we are interested (orange line in Fig (2)).

To study the dependency with the tunnelling we have assumed that both the spin-flip and spin-conserving rates are proportional to each other  $\lambda_i \propto \tau$ , specifically we have used  $\lambda_2 = 0.25\tau$  and  $\lambda_1 = \lambda_2/100$ . If we want to make a transition between the lowest energy triplet and the singlet occupation singlet we must go from  $(\varepsilon(t_0) + u)/E_Z = -4$  to  $(\varepsilon(t_f) + u)/E_Z = -4$ , this means that there is no dark state that does not populate the  $|S(0,2)\rangle$  in the range of detuning in which we are interest unless the tunnelling parameters are high enough. This is why we will try to apply the FAst QUasi ADiabatic (FAQUAD) protocol in Sec. 4.1.

### 3 Triple Quantum Dot

For the system of a linear triple quantum dot array populated with one hole we must work in a Hilbert space of dimension six. Using the Hubbard model in Eq. (1) we can

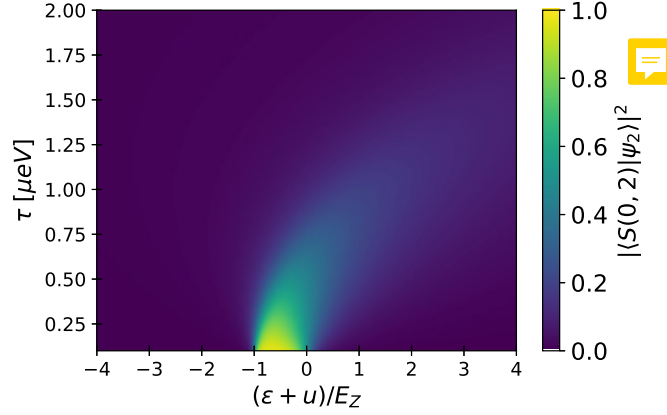


Figure 3: Contribution of the double occupation singlet state in the instant eigenstate  $|\psi_2\rangle$  in terms of the detuning and the spin conserving tunnelling parameter  $\tau$ . For the SOC parameters we have set  $\lambda_1 = \lambda_2/100$  and  $\lambda_2 = 0.25\tau$ .

describe the system with the matrix

$$H = \begin{pmatrix} |\uparrow, 0, 0\rangle & |\downarrow, 0, 0\rangle & |0, \uparrow, 0\rangle & |0, \downarrow, 0\rangle & |0, 0, \uparrow\rangle & |0, 0, \downarrow\rangle \\ \varepsilon_1 + E_Z/2 & 0 & -\tau_{12} & -it_{F,12} & 0 & 0 \\ 0 & \varepsilon_1 - E_Z/2 & -it_{F,12} & -\tau_{12} & 0 & 0 \\ -\tau_{12} & it_{F,12} & \varepsilon_2 + E_Z/2 & 0 & -\tau_{23} & it_{F,23} \\ it_{F,12} & -\tau_{12} & 0 & \varepsilon_2 - E_Z/2 & it_{F,23} & -\tau_{23} \\ 0 & 0 & -\tau_{23} & -it_{F,23} & \varepsilon_3 + E_Z/2 & 0 \\ 0 & 0 & -it_{F,23} & -\tau_{23} & 0 & \varepsilon_3 - E_Z/2 \end{pmatrix}. \quad (9)$$

We have already include the spin-orbit coupling as a tunnelling term between neighbouring QD that flip the spin of the particle. Diagonalizing the matrix we obtain two states that do not populate the middle QD, one of them is

$$|\phi_{1,DS}\rangle = \mathcal{N} \left\{ \frac{1}{t_{F,12}^2 + \tau_{12}^2} [-(\tau_{12}\tau_{23} + t_{F,12}t_{F,23}) |\uparrow, 0, 0\rangle + i(t_{F,23}\tau_{12} - t_{F,12}\tau_{23}) |\downarrow, 0, 0\rangle] + |0, 0, \uparrow\rangle \right\}, \quad (10)$$

where the  $\mathcal{N}$  denoted the normalization factor. This expression can be dramatically simplified considering that the spin flip tunnelling is proportional to the spin-conserving one  $t_F = \tau x$ , then we have

$$\begin{aligned} |\phi_{1,DS}\rangle &= \mathcal{N} \left\{ \frac{\tau_{12}\tau_{23}}{\tau_{12}^2(1+x^2)} [-(1+x^2) |\uparrow, 0, 0\rangle + i(x-x) |\downarrow, 0, 0\rangle] + |0, 0, \uparrow\rangle \right\} \\ &= \left( -\frac{\tau_{23}}{\tau_{12}} |\uparrow, 0, 0\rangle + |0, 0, \uparrow\rangle \right) / \sqrt{(\tau_{23}/\tau_{12})^2 + 1} \\ &= -\sin \theta |\uparrow, 0, 0\rangle + \cos \theta |0, 0, \downarrow\rangle. \end{aligned} \quad (11)$$

We have defined the parameter  $\tan \theta \equiv \tau_{23}/\tau_{12}$ . This is exactly the same dark state that we found in TQD populated with electrons[1], that is, in absence of SOC. Our aim is to transfer a hole from the left quantum dot to the other one throughout the

state<sup>1</sup>

$$|\Psi(t)\rangle = \cos \chi \cos \eta |\uparrow, 0, 0\rangle - i \sin \eta |0, \uparrow, 0\rangle - \sin \chi \cos \eta |0, 0, \uparrow\rangle . \quad (12)$$

In order to apply the inverse engineering protocol to the system we will solve the Schrödinger equation without SOC, obtaining the equations

$$\begin{aligned} \dot{\chi} &= \tan \eta (\tau_{12} \sin \chi + \tau_{23} \cos \chi) \\ \dot{\eta} &= \tau_{12} \cos \chi - \tau_{23} \sin \chi . \end{aligned} \quad (13)$$

The bounding conditions are  $\chi(0) = 0$ ,  $\chi(t_f) = \pi/2$ ,  $\eta(0) = \eta(t_f) = 0$ . Imposing that the pulses must be smooth we have more bounding conditions given by  $\dot{\chi}(0) = \dot{\chi}(t_f) = \ddot{\chi}(0) = \ddot{\chi}(t_f) = 0$  and  $\dot{\eta}(0) = \dot{\eta}(t_f) = 0$ . Our ansatz for these functions will be

$$\begin{aligned} \chi &= \frac{\pi t}{2t_f} - \frac{1}{3} \sin\left(\frac{2\pi t}{t_f}\right) + \frac{1}{24} \sin\left(\frac{4\pi t}{t_f}\right) \\ \eta &= \arctan(\dot{\chi}/\alpha_0) . \end{aligned} \quad (14)$$

Now we can obtain the time dependency of the pulses just by solving Eq. (13). It can be proven that the maximum population of the middle quantum dot is given at  $t = t_f/2$ , and the probability is

$$P_{2,\max} = \frac{16\pi^2}{16\pi^2 + 9t_f^2\alpha_0^2} . \quad (15)$$

As expected, the population of the middle state decreases with the final time. The longer the protocol, the closer we get to an adiabatic transition. The pulses obtained are given in Fig (4).

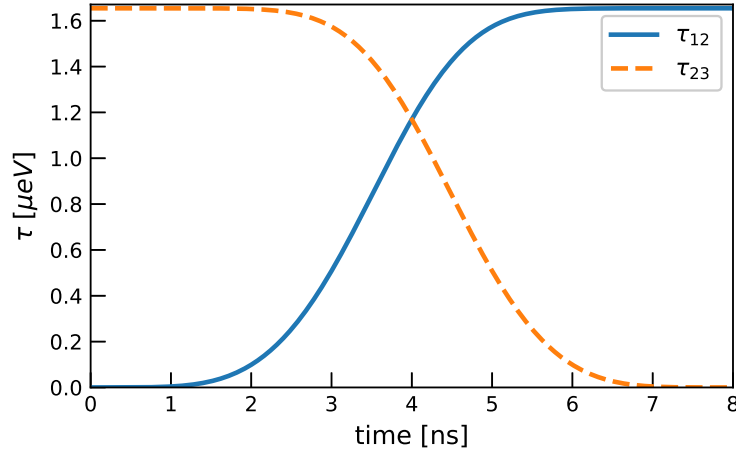


Figure 4: Pulses obtained for the application of the shortcuts to adiabaticity. The parameters used is  $t_f = 8$  ns and  $\alpha_0 = 400$  ns<sup>-1</sup>.

To compute the dynamic of the system we will include the SOC terms. This will give us a different population than our ansatz in Eq. (12), but we will see that the

<sup>1</sup>TO DO: Try to solve the Schrödinger equation with SOC and throughout the state  $|\Psi(t)\rangle = \dots - 1/\sqrt{2} \sin \eta (|0, \uparrow, 0\rangle + |0, \downarrow, 0\rangle) + \dots$

difference is just a population of the state  $|0, \downarrow, 0\rangle$ . The result is plotted in Fig (5). The maximum population in the middle dot, summing the two possible spin configurations, is  $6.6 \times 10^{-4}$ , which is very close to the value given by Eq. (15) of  $6.8 \times 10^{-4}$ . We have obtained a lower population in the middle dot due to the non-vanishing probabilities  $|\downarrow, 0, 0\rangle^2 = |0, 0, \downarrow\rangle^2 \sim 10^{-4}$ . The fidelity obtained is very close to the unity

$$1 - \mathcal{F} \equiv 1 - |\langle \Psi(t_f) | 0, 0, \uparrow \rangle|^2 \sim 10^{-9}. \quad (16)$$

The intensity of the pulses is controlled with the parameters  $\alpha_0$ , the larger it's value,

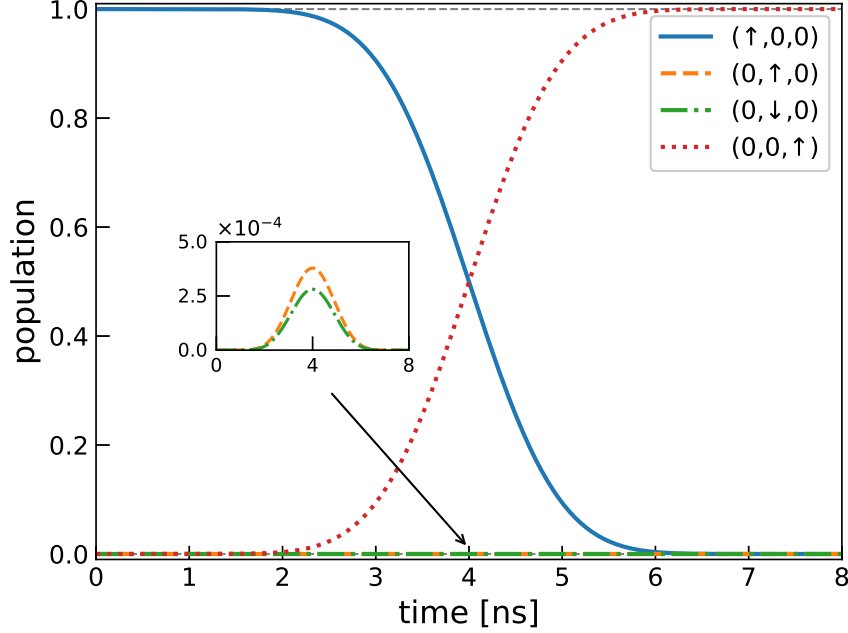


Figure 5: Result for the shortcuts to adiabaticity applied to a TQD system populated with 1 HH which has a non-negligible SOC  $t_F = 0.4 \times \tau$ . The parameter of the protocol is  $\alpha_0 = 400$  ns.

th more intense must be the tunnellings. If this parameters is lower enough we can see that the states  $|\downarrow, 0, 0\rangle$  and  $|0, 0, \downarrow\rangle$  also obtain a non-negligible population Fig (6). In this case the population of the undesired states rises up to a value of  $1 \times 10^{-3}$ , but the fidelity of the protocol remains constant.

## 4 FAQUAD

The standard adiabaticity parameters is imposed to be constant, as

$$\hbar \left| \frac{\langle \phi_1(t) | \partial_t \phi_2(t) \rangle}{E_1(t) - E_2(t)} \right| = c. \quad (17)$$

This is only the case in which there is two states. If we try to include more states the above equation is rewritten as

$$\hbar \sum_{k \neq i} \left| \frac{\langle \phi_i(t) | \partial_t \phi_k(t) \rangle}{E_i(t) - E_k(t)} \right| = c, \quad (18)$$

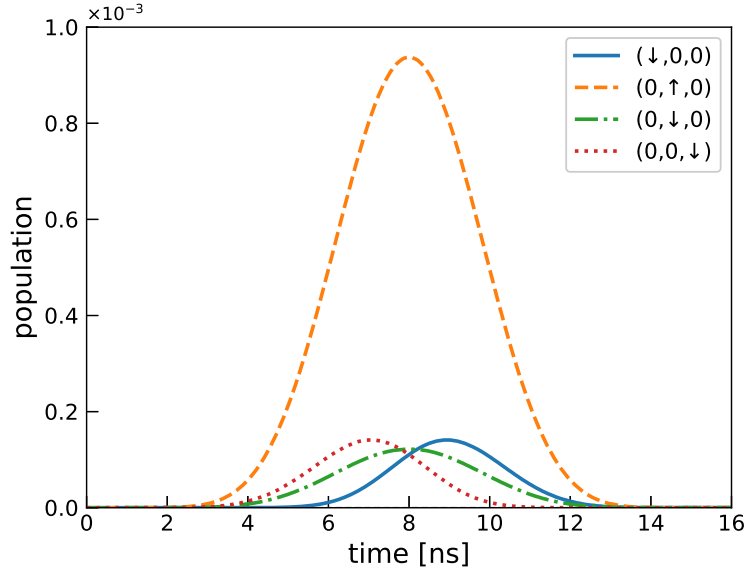


Figure 6: Population of the non-target states in the protocol shortcuts to adiabaticity applied to a TQD system populated with 1 HH. The parameters are  $\alpha_0 = 200$  ns and  $t_f = 16$  ns. Note that the initial and final states are not shown in this figure.

where the index  $i$  denote the state in which we initialize the system, in our case it will be  $|\phi_i(t)\rangle = |T_-(1,1)\rangle$ . Using the chain rule we can write  $\partial_t = \partial_\varepsilon \dot{\varepsilon}$  and the adiabatic condition is then

$$\dot{\varepsilon} = \frac{c}{\hbar} \left( \sum_{k \neq i} \left| \frac{\langle \phi_i(t) | \partial_t \phi_k(t) \rangle}{E_i(t) - E_k(t)} \right| \right)^{-1}. \quad (19)$$

We can rescale the total operation time  $t_f$  to  $s \equiv t/t_f$  and define  $\tilde{c} \equiv ct_f$ , allowing us to write

$$\tilde{c} = \int_{\varepsilon(0)}^{\varepsilon(t_f)} d\varepsilon \left( \sum_{k \neq i} \left| \frac{\langle \phi_i(t) | \partial_t \phi_k(t) \rangle}{E_i(t) - E_k(t)} \right| \right), \quad (20)$$

what can be easily computed numerically, obtaining a value of  $\tilde{c} = 3.79$  ns, so with typical times of  $t_f \sim 10$  ns the adiabaticity parameters obtained is  $c \sim 0.4 < 1$  fulfilling the adiabatic condition. Once we have obtained the value for this parameters, which will remain constant, we can numerically solve the EDO for the evolution of the detuning Eq. (19). The result is shown in Fig. 7, the dependency of this parameters with  $s = t/t_f$  is plotted in a), while its derivative is represented in b) in terms of the detuning. We observe that when we reach the two avoided crossings the rate of change in the detuning decrease significantly, allowing an adiabatic passage, while in the rest of the point the velocity increase in order to speed up the transference process.

#### 4.1 $T_-(1,1) \rightarrow S(1,1)$ in DQD

We define the fidelity of this protocol as

$$\mathcal{F} \equiv |\langle S(1,1) | \psi(t_f) \rangle|^2. \quad (21)$$

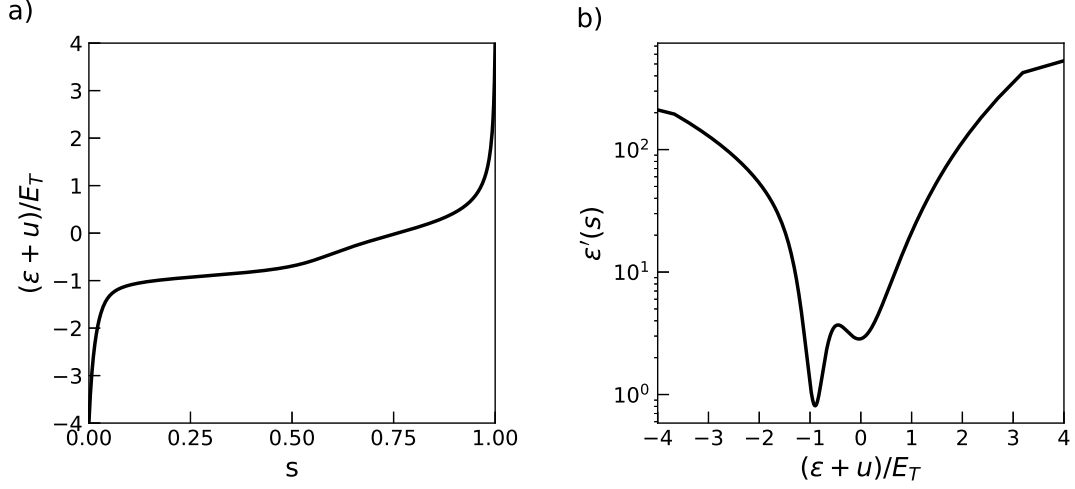


Figure 7: Result obtained for the detuning after applying the FAQUAD protocol to the system of DQD populated with two HH. In a) the dependence of the detuning in terms of the adimensional parameters  $s$ . In b) the slope of the detuning  $\varepsilon' \equiv d\varepsilon/ds$  in terms of the detuning.

Computing this fidelity for different total times  $t_f$  we obtain the results shown in Fig. 8.

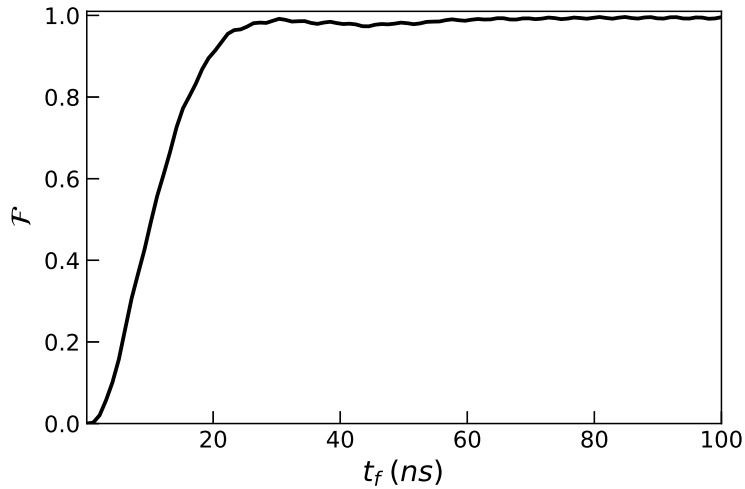


Figure 8: Result for the fidelity in terms of the total time of the protocol.

We can observe that the fidelity shows its typical FAQUAD protocol **swaying** behaviour, reaching a value close to the unit for large enough final times. The first peak is reached at  $t_f = 30.4$  ns, with a fidelity of  $\mathcal{F} = 0.992$ . In Fig. 9 we plot the time evolution for the three different states for this value for the total operation time. We observe that the desired final state is obtained, but in the intermediate times the population for the  $S(0,2)$  state is too high.



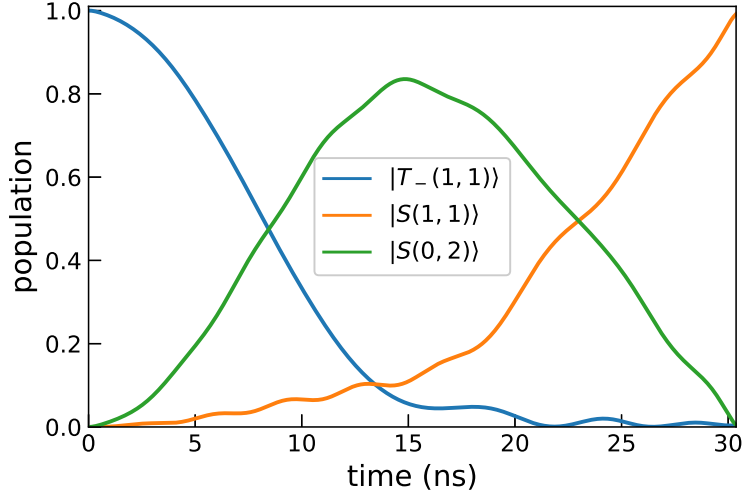


Figure 9: Evolution of the different states for the final time of  $t_f = 30.4$  ns and a fidelity  $\mathcal{F} = 0.992$ .

## A Equivalence between SOC Models

In Sec. 2 we have introduced the SOC with the terms

$$\begin{aligned}\lambda_1 &= \langle T_-(1, 1) | H_D + H_S | S(1, 1) \rangle \\ \lambda_2 &= \langle T_-(1, 1) | H_D + H_S | S(0, 2) \rangle ,\end{aligned}\quad (22)$$

and the total Hamiltonian is then written as

$$H = \begin{pmatrix} |T_-(1, 1)\rangle & |S(1, 1)\rangle & |S(0, 2)\rangle \\ -E_Z & \lambda_1 & \lambda_2 \\ \lambda_1 & 0 & \sqrt{2}\tau \\ \lambda_2 & \sqrt{2}\tau & \varepsilon + u \end{pmatrix}. \quad (23)$$

Supposing Gaussian shapes for the wave functions, and with some given parameters we have obtained that  $\lambda_1 \ll \lambda_2$ . In other references [2] the result is a little different. Using the Loewdin procedure we can redefine our basis orbitals as  $|\bar{L}\rangle = |L\rangle - \frac{1}{2}S|R\rangle$  and  $|\bar{R}\rangle = |R\rangle - \frac{1}{2}S|L\rangle$ , where  $S = \exp(-d^2/2l^2)$  is the overlapping of the original orbitals. Using this we obtain the expression for the spin flip tunnelling

$$\langle \bar{L} \uparrow | H_D + H_S | \bar{R} \downarrow \rangle = -\alpha E_\perp \frac{d^3}{l^6} \exp\left(-\frac{d^2}{2l^2}\right) - i\beta \left(\frac{4d}{l^4} - \frac{d^3}{l^6}\right) \exp\left(-\frac{d^2}{2l^2}\right). \quad (24)$$

We will define this matrix element as  $\langle \bar{L} \uparrow | H_{\text{SOC}} | \bar{R} \downarrow \rangle \equiv -it_F e^{i\delta}$ , where the phase depends on the relative strength of the Rashba and Dresselhaus SOC. With this the Hamiltonian, in the atomic base, is written as

$$H_{\text{atomic}} = \begin{pmatrix} |\uparrow, \uparrow\rangle & |\uparrow, \downarrow\rangle & |\downarrow, \uparrow\rangle & |\downarrow, \downarrow\rangle & |0, \uparrow\downarrow\rangle \\ E_Z & 0 & 0 & 0 & it_F e^{-i\delta} \\ 0 & 0 & 0 & 0 & -\tau \\ 0 & 0 & 0 & 0 & \tau \\ 0 & 0 & 0 & -E_Z & -it_F e^{i\delta} \\ -it_F e^{i\delta} & -\tau & \tau & it_F e^{-i\delta} & \varepsilon + u \end{pmatrix}. \quad (25)$$

Just by changing to the molecular base we obtain the matrix

$$H_{\text{molecular}} = \begin{pmatrix} |T_+(1,1)\rangle & |T_0(1,1)\rangle & |T_-(1,1)\rangle & |S(1,1)\rangle & |S(0,2)\rangle \\ E_Z & 0 & 0 & 0 & it_F e^{-i\delta} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -E_Z & 0 & -it_F e^{i\delta} \\ 0 & 0 & 0 & 0 & -\sqrt{2}\tau \\ -it_F e^{i\delta} & 0 & it_F e^{-i\delta} & -\sqrt{2}\tau & \varepsilon + u \end{pmatrix}. \quad (26)$$

We can restrict ourselves to the subspace  $|T_-(1,1)\rangle, |S(1,1)\rangle, |S(0,2)\rangle$ , computing the characteristic polynomial we have the equation

$$(\varepsilon + u - x)x^2 + x((\varepsilon + u - x)E_Z + t_F^2) + 2(x + E_Z)\tau^2, \quad (27)$$

which does not depend on the exact phase of the spin flip tunnelling, so we can set it to zero  $\delta = 0$ . With this we can write the Hamiltonian for the sub-**scape** in which we are interested as

$$H = \begin{pmatrix} |T_-(1,1)\rangle & |S(1,1)\rangle & |S(0,2)\rangle \\ -E_Z & 0 & -it_F \\ 0 & 0 & \sqrt{2}\tau \\ it_F & \sqrt{2}\tau & \varepsilon + u \end{pmatrix}. \quad (28)$$

This is indeed the same Hamiltonian that the one shown in Eq. (23) under  $\lambda_1 \rightarrow 0$  and  $\lambda_2 \rightarrow -it_F$ .

## References

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