Dephasing and Hyperfine Interaction in Carbon Nanotubes
Double Quantum Dots: The Clean Limit
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We consider theoretically $^{13}$C-hyperfine interaction induced dephasing in carbon nanotubes double quantum dots with curvature induced spin-orbit coupling. For two electrons initially occupying a single dot, we calculate the average return probability after separation into the two dots, which have random nuclear-spin configurations. We focus on the long time saturation value of the return probability, $P_\infty$. Because of the valley degree of freedom, the analysis is more complex than in, for example, GaAs quantum dots, which have two distinct $P_\infty$ values depending on the magnetic field. Here the prepared state and the measured state is non-unique because two electrons in the same dot are allowed in six different states. Moreover, for one electron in each dot sixteen states exist and therefore are available for being mixed by the hyperfine field. The return probability experiment is found to be strongly dependent on the prepared state, on the external magnetic field---both Zeeman and orbital effects—and on the spin-orbit splitting. The lowest saturation value, being $P_\infty = 1/3$, occurs at zero magnetic field for nanotubes with spin-orbit coupling and the initial state being the groundstate, this situation is equivalent to double dots without the valley degree of freedom. In total, we report nine dynamically different situations that give $P_\infty = 1/3$, 3/8, 2/5, 1/2 and for valley anti-symmetric prepared states in an axial magnetic field, $P_\infty = 1$. When the groundstate is prepared the ratio between the spin-orbit splitting and the Zeeman energy due to a perpendicular magnetic field can tune the effective hyperfine field continuously from being three dimensional to two dimensional giving saturation values from $P_\infty = 1/3$ to 3/8.

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I. INTRODUCTION

Quantum dots are attractive candidates for implementing qubits; in particular carbon-based materials such as nanotubes (CNTs) and graphene provide the advantage of a weaker hyperfine interaction. In general the samples have high concentration of $^{12}$C isotopes (spin zero) and low concentration of $^{13}$C isotopes (spin-1/2), and thus the coupling between the confined electron spin and the nuclei spins is small. However, the valley degree of freedom increases the number of available few-particle states in the quantum dots, leading to a more complex system, as compared to, e.g., GaAs quantum dots. Breaking of this 4-fold spin and valley degeneracy has been predicted for nanotubes due to a curvature-induced spin-orbit coupling,\textsuperscript{1–4} which has been confirmed experimentally.\textsuperscript{5–7} The spin-orbit split spectrum leads to doubly degenerate states that can be used as qubit states. For example, by taking advantage of the strong diamagnetic effects in an axial magnetic field, a spin qubit at larger magnetic fields can be defined.\textsuperscript{8} Alternatively, the low field spin-orbit entangled Kramers pair can be used as the qubit, which has been proposed as an electrically manipulatable qubit in bend nanotubes.\textsuperscript{9}

As pointed out by Loss and DiVincenzo,\textsuperscript{10} one of the requirements for quantum dot-based quantum computation is the ability to control the exchange interaction, which has been successfully demonstrated in GaAs double quantum dot (DQD) setups.\textsuperscript{11,12} Similar devices have more recently been fabricated in CNT systems,\textsuperscript{13} which have also attracted considerable theoretically attention.\textsuperscript{14–17}

Another key requirement is long decoherence times. Experimental determination of the spin decoherence times in DQD is done by converting the spin information into charge information, which can be measured using on-chip charge detectors. The charge state of the DQD is characterized by the number of electrons in the left and in the right dot, $(N_L, N_R)$, which are controlled by gate voltages applied to the left and to the right dot, $V_L$ and $V_R$, producing a map of the equilibrium charge states of the double quantum dot, as illustrated in Fig.1(a). The figure also shows the cycle that allows measurement of the dephasing time. This is done by initially preparing the system in a state with two electrons in one dot, then separating them for a certain time with one electron in each dot—while the initial state can be affected by the environment—and finally by measuring the probability for the electrons to return to the original dot.

In this paper, we study the return probability experiment, which measures the characteristic decay time, $T_2^*$, for the return probability averaged over many cycles, as well as the saturation value, $P_\infty$, see Fig.1(b). In the case when the dominant time evolution is due to hyperfine interaction with a nuclear spin background that changes between cycles, the $T_2^*$ time is a measure of the inhomogeneous broadening of the spin state. This is well-studied in two-dimensional electron gases defined quan-
FIG. 1. Return probability experiment. (a) Cycle applied in gate voltage space ($V_L$, $V_R$) in each single-shot measurement. (b) Sketch of the return probability, $P(\tau_s)$, as a function of the time waited, $\tau_s$, at “e”; the saturation value, $P_\infty$, and the decaying time, $\tau_d$, are included. (c) Spectrum of the (1,1) and (0,2) two-particle states (taken for $\Delta_m \neq 0$, tunneling gap, $\Delta_t$, hyperfine characteristic energy, $\sigma_h$, and $B = 0$) as a function of the detuning, $\varepsilon$, arrows and detuning values, $\varepsilon_p$, $\varepsilon_c$ and $\varepsilon_m$ refer to the single-shot cycle’s stages presented in (a). We label with squares (“e.g.”) the states that the system may occupy at the stages, “p”, “e” and “m” if the (0,2) highest energy excited state is prepared; the possible outcomes at $\varepsilon_m$ would be different if the prepared state, $|\psi_0\rangle$, had been one of the other five available (0,2) states.

Considered did not, however, involve valley mixing terms in contrast to the C-based dots we treat here. The motivation of our detailed study is to predict the expected return probabilities for carbon based systems with hyperfine coupling to spin $1/2$ $^{13}$C nuclei. In these graphene-based systems, in contrast to Si double dots, one must take into account that the hyperfine interaction affects both the spin and the valley degrees of freedom. We include those hyperfine valley mixing effects but we do not include disorder induced spin conserving valley mixing, which is presented in a separate publication. Furthermore, we include direct Coulomb interaction, but not Coulomb exchange which is expected to be a small effect.

We also work in the limit of large detuning so that the tunneling exchange on the (1,1) states is much smaller than the hyperfine field characteristic energy and therefore we obtain the lower bounds for $P_\infty$. On the other hand, if the tunneling exchange is important, the degeneracies for zero hyperfine are reduced diminishing the effectiveness of the hyperfine-induced mixing and therefore also increasing the saturation values of the return probability. In those situations $P_\infty$ grows continuously, as a function of the tunneling exchange, from the zero-exchange value up to one.

We start from a simple model for an isolated quantum dot and construct from this the two-electron wave functions. We study the cases of large and small spin-orbit coupling. The result is found to be dependent on the prepared state and on the external magnetic field. Notably, for some situations the two-electron wave function is almost not dephased by the hyperfine field. We show that besides the usual saturation values of the return probability, $1/3$ and $1/2$—well known in DQDs without the valley degree of freedom and for zero tunneling exchange—other values can be observed; namely, $3/8$, $0.4$ and $1$. In addition, for nanotubes with spin-orbit coupling, an applied magnetic field in a direction perpendicular to the tube axis can tune the saturation value between $1/3$ and $3/8$.

The paper is organized as follows. In section II, we describe the double dot model and the four special cases used in the paper. Section III describes the experiment and the methods used to calculate the return probabilities, with results presented in Section IV. Finally, conclusions and summary are found in Section V.

II. QUANTUM DOT MODEL

A. Single dot

We consider semiconducting tubes where the bandgap is due to either chirality or, for nominally metallic tubes, to curvature. The semiconducting properties allow electrons to be confined in a gate-defined potential, to curvature. This potential is assumed smooth on the scale of the interatomic distance, conserving the valley index. Both single$^8$ and double quantum dots$^{14–16}$ have been studied.
in this approximation. An important effect of curvature in nanotubes is that it leads to spin-orbit interaction that couples the valley index with the spin in the longitudinal direction.\textsuperscript{1–4}

The Hamiltonian describing the spin and valley degrees of freedom, excluding the hyperfine interaction, reads

\[ H_{sv} = H_s + H_v + H_{orb}, \]

where \( H_s \) is the spin-orbit coupling term, \( H_v \) is the Zeeman interaction and \( H_{orb} \) is the diamagnetic effect of the magnetic field. For the specific cases considered below, not all terms in Eq.(1) are present.

The spin-orbit coupling term is

\[ H_{so} = -\frac{1}{2} \Delta_{so} \tau_3 \sigma_\parallel, \]

where \( \Delta_{so} \) is the spin-orbit energy splitting, \( \sigma_\parallel \) is the spin operator along the direction of the tube axis and \( \sigma_x, \sigma_y, \sigma_z \) (\( \sigma_0 \)) and \( \tau_1, \tau_2, \tau_3 \) (\( \tau_0 \)) are the Pauli (identity) matrices in spin and valley space, respectively. For the valley degree of freedom, we use \( \tau = K, K' \) to identify the +1 and −1 eigenstates of \( \tau_3 \). In the following, unless otherwise stated, the spin quantization axis—\( \pm \sigma \) (\( \uparrow, \downarrow \) or equivalently, \( \sigma = \pm \))—is taken along the direction of the total magnetic field. The value of the spin-orbit splitting depends on the nanotube’s chiral vector and on the electron filling.\textsuperscript{7}

The Zeeman energy due to an external magnetic field \( B_{ex} = (B_x, B_y, B_z) \) is

\[ H_s = \frac{1}{2} g_s \mu_B \gamma_0 \left(B_{ex} \cdot \sigma \right), \]

where \( g_s = 2 \) is the usual gyromagnetic factor. The component of the magnetic field parallel to the tube axis, \( B_\parallel \), gives rise to a strong diamagnetic effect:

\[ H_{orb} = g_{orb} \mu_B B_\parallel \gamma_0 \sigma_0, \]

where the orbital g-factor, \( g_{orb} \), depends on the size of the nanotube\textsuperscript{30} and it is bigger than \( g_s/2 \) in the typical case: nanotubes with radius greater than 1 nanometer.\textsuperscript{5–7} To simplify the notation, we define the following two energy scales:

\[ E_s = g_s \mu_B |B_{ex}|, \]

\[ E_{orb} = 2 g_{orb} \mu_B |B_\parallel|. \]

1. Four special cases

Here we identify four special cases of single quantum dots, representing different physical realizations, see also Fig. 2. The important classification is the splitting of the dot state compared with the hyperfine energy. The relevant energy scales are Zeeman splitting, \( E_s \), orbital splitting, \( E_{orb} \), and spin-orbit splitting, \( \Delta_{so} \); we only consider each one of them when they become much bigger than the hyperfine interaction. Based on this, we define:

\[ \begin{align*}
(a) & \quad \Delta_{so} = 0, \quad E_{orb} = 0 \\
(b) & \quad \Delta_{so} = 0, \quad E_{orb} \neq 0 \\
(c) & \quad \Delta_{so} \neq 0, \quad E_{orb} \neq 0 \\
(d) & \quad \Delta_{so} \neq 0, \quad E_{orb} = 0
\end{align*} \]

Case A) No spin-orbit coupling and no orbital magnetism, only the Zeeman energy \( E_s \) is considered. This is relevant for nanotube dots with small spin-orbit energy in a perpendicular magnetic field (so that \( E_{orb} = 0 \)) or, alternatively, graphene dots in an in-plane magnetic field.\textsuperscript{31} The single-particle spectrum as a function of the magnetic field is shown in Fig. 2(a). Results for valley degenerated quantum dots are presented in Sec.IV A.

Case B) Quantum dot with no spin-orbit coupling and finite orbital magnetism; this is the situation for nanotubes with small spin-orbit splitting in a magnetic field with a parallel component. In this case, the energies \( E_s \) and \( E_{orb} \) are both relevant. Figure 2(b) shows
the spectrum as a function of the magnetic field, which breaks the 4-fold degeneracy. Since we have assumed that $E_{orb} > E_s$, which is likely the case if the total magnetic field is parallel to the tube axis,5–7 the two highest energy solutions have $\tau = K$, whereas the two lowest energy solutions have $\tau = K'$. Results for the current case are presented in Sec.IV B.

Case C) Quantum dot in a nanotube with spin-orbit coupling and external magnetic field parallel to the tube axis; all three energy scales $\Delta_{so}, E_s$ and $E_{orb}$ are relevant. At zero magnetic field, in contrast to cases A and B, the spin-orbit coupling breaks the four-fold degeneracy, which results in two Kramers doublet. The energy of the two Kramers doublets are $\pm \Delta_{so}/2$, as shown in 2(c), which depicts the spectrum as a function of the magnetic field. For two finite fields some degeneracies are recovered. Results for this situation are presented in Sec.IV C.

Case D) Here the system has a finite spin-orbit coupling and the magnetic field is perpendicular to the tube axis, therefore, diamagnetic effects are absent. Even for finite Zeeman energy, $E_s$, the doublets are not split because the magnetic field cannot couple opposite valley, see Fig. 2(d). The ratio between $E_s$ and $\Delta_{so}$ controls the spin projection of the solutions; the bigger the magnetic field the more similar to case A the solutions become because the spin of the eigenstates tend to align with the magnetic field. This quantum dot solutions and the return probability results are presented in Sec.IV D.

B. The double dot

The double dot single-particle Hamiltonian is

$$H_{DQD}^{1p} = H_{LR}^{1p} + H_T^{1p},$$

(7)

where $H_{LR}^{1p}$ includes the Hamiltonians for the two isolated dots and $H_T^{1p}$ is the single-particle tunneling between the two dots. In what follows we use the superindex 1p or 2p to distinguish single-particle and two-particle operators. We introduce the Pauli (identity) matrices $\xi_1$ ($\xi_0$) in left-right space, with $\pm 1$ eigenvalues of $\xi_3$ for L/R, respectively.

In this notation, the tunneling part of the Hamiltonian becomes

$$H_T^{1p} = -t\xi_1\tau_0\sigma_0.$$  

(8)

This inter-dot tunneling is assumed to be valley and spin conserving, because the gate voltage defined confining potential is non-magnetic and it is assumed smooth on the lattice scale. We also assume that the tunneling amplitude does not depend on the quantum numbers $\tau$ and $\sigma$, which is valid as long as the height of the potential barrier is much bigger than the detuning, the spin-orbit and magnetic splittings.15,16

The isolated left dot plus right dot single-particle Hamiltonian is

$$H_{LR}^{1p} = \tau_0\sigma_0\frac{\xi_0(\epsilon_L + \epsilon_R) + \xi_3(\epsilon_L - \epsilon_R)}{2} + \xi_0 H_{sv},$$

(9)

where the last term is the valley and spin Hamiltonian in Eq. (1) which is identical in the two quantum dots. The effects of the gate voltages are introduced as the energy shifts $\epsilon_L$ and $\epsilon_R$ for the left and the right dot, respectively.

C. Two-particle basis states, no tunneling

A single-particle basis set can be generated by the eight states $|\xi\tau\sigma\rangle$, with $\xi = L, R$, $\tau = K, K'$ and the spin projection $\sigma = \uparrow, \downarrow$ is taken along the direction of the magnetic field. If $\Delta_{so} = 0$, or if the magnetic field is parallel to the tube’s axis, $|\xi\tau\sigma\rangle$ are eigenstates of the single-particle Hamiltonian $H_{LR}^{1p}$ with eigenenergies

$$E_{\xi\tau\sigma} = (E_{\xi\sigma} + E_{orb}\tau - \Delta_{so}\tau\sigma)/2.$$  

(10)

Using these states we build two-particle Slater determinants with quantum numbers $\xi\tau\sigma$ and $\xi'\tau'\sigma'$ as follows

$$\left|\xi\tau\sigma\right\rangle = \frac{1}{\sqrt{2}} \left( |\xi\tau\sigma\rangle_1 |\xi'\tau'\sigma'\rangle_2 - |\xi'\tau'\sigma'\rangle_1 |\xi\tau\sigma\rangle_2 \right).$$  

(11)

Since the single-particle basis has eight elements, the two-particle basis has 28 states $(28 = 8!/(6!2!))$. However, for the return probability due to energetic reasons we do not include the states with two electrons in the left dot, i.e., the $(2,0)$ charge configuration, which leaves 22 states.

In general, the single-particle eigenstates can differ from $|\xi\tau\sigma\rangle$; we label the single-particle eigenstates of $H_{sv}$ as $|n\rangle$, with energies $E_n$, using the index $n = 1, \ldots, 4$; then, the six $(0,2)$ eigenstates and their eigenenergies are

(0, 2) : $|Rn\rangle, E_{n,n'}^{(0,2)} = 2E_R + E_n + E_{n'} + U_{RR},$  

(12)

where $n, n' = 1, \ldots, 4$ and $n < n'$. Here we included electron-electron interaction, represented by the right dot charging energy $U_{RR}$. We have not included Coulomb exchange since it is expected to be small.7,16 With one electron in each dot the sixteen $(1,1)$ eigenstates and their corresponding eigenenergies are

(1, 1) : $|Ln\rangle, E_{n,n'}^{(1,1)} = \epsilon_L + \epsilon_R + E_n + E_{n'} + U_{LR},$  

(13)

where $U_{LR}$ is the inter-dot Coulomb repulsion.

D. Inter-dot tunneling

The single-particle Hamiltonian of Eq.(8) preserves the spin and valley degrees of freedom in the inter-dot tunneling ($L \leftrightarrow R$), therefore, the tunneling Hamiltonian can be rewritten in terms of the single-particle eigenstates as:

$$H_T^{1p} = -t \sum_{n=1}^{4} \langle Ln | (Rn| + |Rn\rangle (Ln) \rangle.$$  

(14)
When acting with the tunneling Hamiltonian on the (0,2) two-particle basis states it gives,
\[
H_{T}^{2p} \left( \left| R_{n}^{n'} \right> \right) = -t \left( \left| R_{n}^{n'} \right> + \left| L_{n}^{n'} \right> \right),
\]
i.e., a combination of (1,1) Slater determinants associated with those single-particle states. Thus, any given pair \( n, n' \) gives a \( 3 \times 3 \) Hamiltonian. In the basis, \( \left| R_{n}^{n'} \right>, \left| L_{n}^{n'} \right> \), and \( \left| R_{n}^{n'} \right| = \left| L_{n}^{n'} \right>, \) this Hamiltonian matrix becomes
\[
H_{nn'} = E_{AV} + E_{n} + E_{n'} + \begin{pmatrix}
-\varepsilon & -t & -t \\
-t & \varepsilon & 0 \\
-t & 0 & -\varepsilon
\end{pmatrix},
\]
where the detuning, \( \varepsilon \), and the average energy, \( E_{AV} \), have been defined as
\[
\varepsilon \equiv E_{n,n'}^{(1,1)} - E_{n,n''}^{(0,2)} = \epsilon_{L} - \epsilon_{R} - U_{RR} + U_{LR},
\]
and
\[
E_{AV} = \frac{1}{2} \left( E_{n,n'}^{(1,1)} + E_{n,n''}^{(0,2)} - (E_{n} + E_{n'}) \right) = \frac{1}{2} (\varepsilon + 3\epsilon_{R} + U_{LR} + U_{RR}).
\]
For the mixing of the (0,2) and the (1,1) states, the global energy shift \( E_{AV} + E_{n} + E_{n'} \) is irrelevant, and therefore we choose \( E_{AV} = 0 \) from this point on. The Hamiltonian of Eq.(16) can in fact be reduced to a 2 by 2 system because the following (1,1) combination,
\[
\left| LR_{n,n'}^{n,n''} \right> \equiv \frac{1}{\sqrt{2}} \left( \left| R_{n}^{n'} \right> - \left| L_{n}^{n'} \right> \right),
\]
is an eigenstate with energy independent of \( t \), \( E_{n,n',n''}^{(1,1),\text{odd}} = \frac{1}{2} + E_{n} + E_{n'} \). In the Pauli blockade language this is a blocked state. The left-right (LR) symmetry of this state is evident when writing it as a product in LR- and \( nn' \)-spaces:
\[
\left| LR_{n,n'}^{n,n''} \right> = \left| S_{LR} \right> \left| T_{n,n'} \right>,
\]
where we introduced the notation of a “singlet” in LR-space. It is convenient to introduce also the triplet states in this space, and we define
\[
\left| S_{LR} \right> = \frac{1}{\sqrt{2}} \left( \left| R_{1}^{1} \right> \left| L_{2}^{2} \right> - \left| R_{2}^{2} \right> \left| L_{1}^{1} \right> \right),
\]
\[
\left| T_{LR}^{+} \right> = \frac{1}{\sqrt{2}} \left( \left| R_{1}^{1} \right> \left| L_{2}^{2} \right> + \left| R_{2}^{2} \right> \left| L_{1}^{1} \right> \right),
\]
\[
\left| T_{LR}^{-} \right> = \left| R_{1}^{1} \right> \left| L_{2}^{2} \right>,
\]
\[
\left| T_{LR}^{0} \right> = \left| R_{1}^{1} \right> \left| L_{2}^{2} \right>,
\]
Similarly, we have defined singlet-like and triplet-like functions in valley and spin spaces (not shown). Finally, for the combined quantum number \( n \), we define
\[
\left| S_{n,n'} \right> = \frac{1}{\sqrt{2}} \left( \left| n_{1}^{1} \right> \left| n_{2}^{2} \right> - \left| n_{1}^{2} \right> \left| n_{2}^{1} \right> \right),
\]
\[
\left| T_{n,n'} \right> = \frac{1}{\sqrt{2}} \left( \left| n_{1}^{1} \right> \left| n_{2}^{2} \right> + \left| n_{1}^{2} \right> \left| n_{2}^{1} \right> \right).
\]
of the three two-particle states associated with the two single-particle states \(|n\rangle\) and \(|n'\rangle\). Six groups of 3 states with exactly the same energy gap appear, one for each of the possible \(n, n'\) non-equivalent pairs (see Fig.1(c)). The four remaining states (that complete the 22 solutions) are the \((1,1)\) LR-antisymmetric states that arise from Slater determinants constructed with the same single-particle state in both dots:

\[
|\text{R}_n\rangle = |S^{LR}\rangle (|n\rangle_1 |n\rangle_2).
\]

Using spin and valley singlet and triplets functions the states in Eq.(27) can be written (for the quantum dots of case A, B and C: \(\sigma\) is a good quantum number) as the four states with full polarization in spin and valley spaces, i.e., \(|S^{LR}T^{\text{spin}}_{\pm}\rangle\) and \(|S^{LR}T^{\text{spin}}_{\pm}\rangle\).

In summary, there are ten LR-antisymmetric states that do not mix with the \((0,2)\) solutions. Six of them with \(n \neq n'\), as it is shown in Fig.3, become quasi-degenerated with their associated \(n, n'\) LR-symmetric partners at the high detuning limit, i.e., when \(|\varepsilon|/t| \gg 1\). The six LR-symmetric states are connected by inter-dot tunneling to the corresponding \(n, n'\) \((0,2)\) states as follows,

\[
|\text{T}^0_{\text{LR}}\rangle |S_{n,n'}\rangle \leftrightarrow |\text{T}^1_{\text{LR}}\rangle |S_{n,n'}\rangle.
\]

Obviously, as it is seen in detail in the next sections, the connectivity between \((0,2)\) states and \((1,1)\) states plays a key role in the return probability experiment.

\section*{E. Hyperfine coupling}

Taking \(\sigma\) the spin operator of the confined electron in a graphene-based quantum dot, the hyperfine interaction has the following form:

\[
H_{hf} = \sum I_{ls} \chi_{ls} (\Psi^r \Psi^s R_{ls} |\chi_{ls}\rangle).
\]

where \(I_{ls}\) is the isotropic hyperfine coupling constant.

\section*{F. Hyperfine coupling}

Taking \(\sigma\) the spin operator of the confined electron in a graphene-based quantum dot, the hyperfine interaction has the following form:

\[
H_{hf} = \sum I_{ls} \chi_{ls} (\Psi^r \Psi^s R_{ls} |\chi_{ls}\rangle).
\]

where \(I_{ls}\) is the isotropic hyperfine coupling constant.

\section*{G. Hyperfine coupling}

Taking \(\sigma\) the spin operator of the confined electron in a graphene-based quantum dot, the hyperfine interaction has the following form:

\[
H_{hf} = \sum I_{ls} \chi_{ls} (\Psi^r \Psi^s R_{ls} |\chi_{ls}\rangle).
\]

where \(I_{ls}\) is the isotropic hyperfine coupling constant.

\section*{H. Hyperfine coupling}

Taking \(\sigma\) the spin operator of the confined electron in a graphene-based quantum dot, the hyperfine interaction has the following form:

\[
H_{hf} = \sum I_{ls} \chi_{ls} (\Psi^r \Psi^s R_{ls} |\chi_{ls}\rangle).
\]

where \(I_{ls}\) is the isotropic hyperfine coupling constant. 

\section*{I. Hyperfine coupling}

Taking \(\sigma\) the spin operator of the confined electron in a graphene-based quantum dot, the hyperfine interaction has the following form:

\[
H_{hf} = \sum I_{ls} \chi_{ls} (\Psi^r \Psi^s R_{ls} |\chi_{ls}\rangle).
\]

where \(I_{ls}\) is the isotropic hyperfine coupling constant. 

\section*{J. Hyperfine coupling}

Taking \(\sigma\) the spin operator of the confined electron in a graphene-based quantum dot, the hyperfine interaction has the following form:

\[
H_{hf} = \sum I_{ls} \chi_{ls} (\Psi^r \Psi^s R_{ls} |\chi_{ls}\rangle).
\]

where \(I_{ls}\) is the isotropic hyperfine coupling constant.
In terms of these fields, the double dot single-particle HFI Hamiltonian can be written as

$$H^\text{dp}_{h,\text{LR}} = \sum_{ij=0}^{2} \sum_{j=x,y,z} \left( h_j^i \xi_0 + \delta h_j^i \xi_3 \right) \tau_j \sigma_j,$$

(36)

which should be added to the Hamiltonian of the double dot in Eq.(7).

1. Hyperfine field in single valley systems

Here we briefly introduce the key features of the HFI found in single valley systems, e.g., GaAs double dots. The well-known relevant states and the action of the HFI Hamiltonian in those systems is an important reference for comparison. Because the valley space is absent in GaAs, the single-particle Hamiltonian of the hyperfine field interaction is

$$H^\text{dp}_{h,\text{GaAs}} = \sum_{j=x,y,z} \left( h_j^0 \xi_0 + \delta h_j^0 \xi_3 \right) \sigma_j.$$  

(37)

Due to the absence of the orbital degree of freedom there exist four (1,1) states, namely, the spin singlet and triplets,

$$|1, \text{GaAs}\rangle = |T_0^\text{LR-\text{spin}}\rangle, \quad |2, \text{GaAs}\rangle = |S^\text{LR-\text{spin}}\rangle,$$

$$|3, \text{GaAs}\rangle = |S^\text{LR-\text{spin}}\rangle, \quad |4, \text{GaAs}\rangle = |T_0^\text{LR-\text{spin}}\rangle.$$  

(38)

The HFI Hamiltonian of Eq.(37), written in the latter basis, becomes

$$H^\text{GaAs}_{h} = \left( \begin{array}{ccc}
0 & \delta z & \delta x y^* & \delta x y \\
\delta z & 0 & \pi y & \pi y \\
-\delta x y & \pi y & 0 & -\pi \\
\delta x y^* & \pi y & 0 & -\pi
\end{array} \right),$$

(39a)

$$\delta z \mapsto 2 \delta h_z, \quad \pi \mapsto 2 \pi,$$

(39b)

$$\delta x y \mapsto \sqrt{2} (\delta h_x - i \delta h_y), \quad \pi y \mapsto \sqrt{2} (\pi x - i \pi y).$$

(39c)

One sees that only the inhomogeneous HFI is able to mix the LR-symmetric function (spin singlet) with the LR-antisymmetric (spin-triplets) functions. In particular the $\delta h_z$ component also conserves the total $S_z$ and therefore is able to mix the $|T_0^\text{LR-\text{spin}}\rangle$ with the $|S^\text{LR-\text{spin}}\rangle$. In the next section we show that some specific situations in CNT double dots can be mapped to the Hamiltonian of Eq.(39a) or to a modified version of it.

III. SIMULATING THE EXPERIMENT

The return probability, $P(\tau_\circ)$, for a given evolving time, $\tau_\circ$, see Fig.1(b), is obtained experimentally by averaging over a set $\{i = 1, 2, \ldots, N\}$ of single shot measurements with outcomes $O_i, \tau_\circ$.

$$P(\tau_\circ) = \frac{1}{N} \sum_{i=1}^{N} O_i, \tau_\circ.$$

(40)

Each single-shot measurement consists of a gate-voltage cycle with five stages (see arrows and points “p”, “e” and “m” in Fig. 1(a) and the associated detuning values $\varepsilon_p$, $\varepsilon_e$ and $\varepsilon_m$ in Fig. 1(c)).

(i) **Preparation**, the DQD is prepared in the (0,2) region at point “p”.

(ii) **Separation**, by applying a voltage pulse of length $\Delta \varepsilon$ and duration $T_S$, which is short on the scale of the HFI interaction ($T_S \ll \frac{\pi}{2\delta}$), but slow on the scale of the inverse tunneling energy, the initial (0,2) state is adiabatically moved to the point “e” deep into the (1,1) region. If the detuning is changed by $\Delta \varepsilon > t$, the condition for adiabatic conversion is $T_S > h \Delta \varepsilon / t^2$.

(iii) **Evolution**, the system is left to evolve at the point “e” during a time $\tau_\circ$; in this stage the electron wavefunction in each dot acquires a different dynamical phase due to the hyperfine coupling with the nuclei spins; in general, the system oscillates between the initial (1,1) wavefunction and other combination of (1,1) states.

(iv) **Joining**, a voltage pulse brings the system back to the (0,2) region; with the same adiabatic condition as for the separation stage.

(v) **Measuring**, at the “m” point a nearby charge sensing device determines the outcome $O_i, \tau_\circ$ (1 or 0) of the single shot measurement; $O_i, \tau_\circ$ is set to 1 only when the system has returned to an (0,2) configuration.

Depending on the preparation protocol the initial (0,2) state can be different than the ground state. We cover all the possibilities by assuming a prepared state in an arbitrary superposition of the six possible zero-hyperfine (0,2) eigenstates, $|\psi_\circ\rangle = \sum_l a_l |l, (0,2)\rangle$, where each $|l, (0,2)\rangle$ state is one of the six Slater determinants given in Eq.(12). When averaging the outcomes $O_i, \tau_\circ$ of a large number of single-shot measurements over an ensemble of random hyperfine field, the phases of $a_l$ average out and the resulting probability for a given initial state is simply given by

$$P_{\psi_\circ}(\tau_\circ) = \sum_l |a_l|^2 P_l(\tau_\circ),$$

(41)

where $P_l(\tau_\circ)$ is the return probability when starting in the (0,2) eigenstate $|l, (0,2)\rangle$. Therefore, the return probability of a general case can be evaluated by knowing the values $|a_l|$ and the return probabilities obtained when preparing the (0,2) zero-hyperfine eigenstates separately.

For these reasons, in each of the DQD scenarios that we deal over the next sections, we focus on the behaviour of the six functions, $P_l(\tau_\circ)$.

Due to its experimental importance we focus the discussion on the saturation value of the return probability which is defined as

$$P_\infty \equiv \lim_{\tau_\circ \to \infty} P(\tau_\circ).$$

(42)

In addition, we define the decaying time, $\tau_d$, as the time for which

$$P(\tau_d) = \frac{1}{2} P_\infty + \frac{1}{2}.$$

(43)
see Fig.1(b).

In general, \( P(\tau_s) \) may be different when the hyperfine field of the two dots follow Gaussian distributions with different rms values, \( \sigma_{h1}^L \) and \( \sigma_{h1}^R \). In fact, this is the case when the numbers of 13C atoms are different for the left and right dots (see Eq.(30)). However, this would affect the transient of \( P(\tau_s) \) but not the behavior for \( \tau_s \to \infty \). In this work we focus on the saturation values and on transient features intrinsic to DQDs in C-based systems. For this reason we choose \( \sigma_{h1}^L = \sigma_{h1}^R \equiv \sigma_h \) in the following.

A. Numerical evaluation of the return probabilities

We have developed a numerical simulation of the experimental cycle outlined above. The time evolution inside the (1,1) region (point “\( e \)” in Fig.1(a)) is governed by the hyperfine field alone, i.e., it is assumed that \( t^2/\Delta \varepsilon \ll \sigma_h \). Essentially, as discussed in the introduction, we are working in the large detuning limit where the effect of the tunneling exchange is negligible and therefore we are able to obtain the lower bounds of the saturation return probabilities. For solving such a time evolution we start with the LR-symmetric (1,1) state, \( |LR_{n,n''}\rangle \), which is connected (see Eq.(28)) with the (0,2) prepared state \( |\psi_0\rangle \); this is then decomposed into the numerically determined eigenstates of the 16 by 16 Hamiltonian for the current hyperfine field realization (generated following the Gaussian distributions with variances given in Eq.(30)), and hence the time dependent (1,1) state can be computed as a superposition of time-evolved eigenstates.

To calculate the return probability, we define an operator that projects onto LR-symmetric states as

\[
\hat{P}_{LR-sym} \equiv |T_{0}^{LR}\rangle \langle T_{0}^{LR}|. \tag{44}
\]

The return probability after time \( \tau_s \) for a given hyperfine field realization \( \tau_r \) is then

\[
p_{r_s}(\tau_s) = \langle \Psi_r(\tau_s) | \hat{P}_{LR-sym} | \Psi_r(\tau_s) \rangle. \tag{45}
\]

The projection method assumes the joining stage (iv) is performed under the same adiabatic conditions as the separating stage (ii). After repeating this procedure for a large number of realizations, \( N_r \), the final return probability \( P(\tau_s) \) is obtained by averaging

\[
P(\tau_s) = \frac{\sum_{r=1}^{N_r} p_{r_s}(\tau_s)}{N_r}. \tag{46}
\]

B. Analytical evaluation of the return probability

For analytic evaluation of the return probability, we use the same set of conditions as for the numerical evaluation, namely that the time evolution after the separation stage is only governed by hyperfine interaction (i.e., no tunneling exchange), and that the return probability after evolution can be computed by projection. In this high detuning limit—excluding for the moment the HFI effect— the LR-symmetric states can be considered degenerated with their LR-antisymmetric partners (see Fig.3 and Eq.(13)). Additional degeneracies are determined by presence of spin-orbit coupling and applied magnetic field. We assume that with finite spin-orbit coupling and/or applied magnetic field the hyperfine interaction only mixes states within the subset of quasi-degenerate states.

Due to the LR-symmetry, since the evolution starts in a LR-even state, the degeneracies of the subspaces of evolution in (1,1) are never lower than two. In this paper degeneracies \( n_e = 2, 3, 4, 8 \) and 16 appear. To determine the time evolution, we project the Hamiltonian to the (1,1) subspace connected with the prepared (0,2) state, the reduction of the system—if any—sometimes allows analytical treatment. Then, we focus on the form and the statistical properties (i.e., variances) of the surviving mixing terms of the HFI Hamiltonian. Those matrix elements are obtained by elementary calculations; the (1,1) basis expanded using singlet and triplet functions in LR, valley and spin spaces (instead of the Slater determinant basis) is useful for a more direct physical interpretation of the hyperfine mixing terms.

C. State counting estimation of \( P_\infty \)

Here we introduce a scheme for estimating the return probability based on a simple state counting argument. The value obtained with the procedure that follows does not always coincide with the exact value, \( P_\infty \), however it is useful for visualizing special features of the exact dynamics. In order to compute the state counting value, first, we find the number of degenerate (1,1) states, \( n_e \), connected with the chosen (0,2) prepared state under investigation. Second, we find the number of LR-symmetric states, \( n_{(0,2)} \), connected with that (1,1) subspace of \( n_e \) states, \( S_c \). Third, assuming a fully incoherent mixing of the initial state with all states, for \( \tau_s \to \infty \) every one of the \( n_e \) states should have a probability \( 1/n_e \) of being occupied, therefore, the estimated return probability becomes

\[
P_\infty \equiv \frac{n_{(0,2)}}{n_e}. \tag{47}
\]

One can expect this to be a lower bound for \( P_\infty \), because under coherent evolution the system does not fully randomize and might therefore maintain a larger weight on the initial state which is connected. This is the case for example in GaAs double dots, whereas the estimation gives \( P_\infty = 1/4 \), the coherent evolution (averaged over many realizations) gives \( P_\infty = 1/3 \).
IV. RESULTS

1. Labeling of the energy levels

With the exception of Sec.IV D (case D), in the following, the single-particle eigenstates in each dot are \( |\xi, n\rangle \) with \( |n\rangle = |\sigma\rangle \), where \( \sigma \) is the spin projection along the direction of the applied magnetic field taken, for convenience, along the \( z \)-direction. The two-particle functions \( |S_{n,n'}\rangle \) and \( |T_{n,n'}\rangle \) presented in Eqs. (22) can be further expanded in terms of tensor products in spin and valley spaces. The procedure is straightforward and states \( |S_{n,n'}\rangle \) and \( |T_{n,n'}\rangle \) are found to be equivalent to a unique tensor product in valley and spin except for \( n, n' \equiv K \uparrow, K' \downarrow \) and \( n, n' \equiv K \downarrow, K' \uparrow \) in which case they are given by,

\[
|S_{K\uparrow,K'\downarrow}\rangle = \frac{1}{\sqrt{2}} \left( |S_{val}^0 T_{0}^{spin}\rangle + |T_{0}^{val} S_{spin}\rangle \right), \quad (48a)
\]

\[
|T_{K\uparrow,K'\downarrow}\rangle = \frac{1}{\sqrt{2}} \left( |T_{0}^{val} S_{spin}\rangle + |S_{spin} T_{val}^0\rangle \right), \quad (48b)
\]

\[
|S_{K \downarrow, K' \uparrow}\rangle = \frac{1}{\sqrt{2}} \left( |S_{val}^0 T_{0}^{spin}\rangle - |T_{0}^{val} S_{spin}\rangle \right), \quad (48c)
\]

\[
|T_{K \downarrow, K' \uparrow}\rangle = \frac{1}{\sqrt{2}} \left( |T_{0}^{val} S_{spin}\rangle - |S_{spin} T_{val}^0\rangle \right). \quad (48d)
\]

These states are particularly important in the presence of spin-orbit coupling.8,14,16,37 For the sake of readability in the following we sometimes omit the ket symbol, \( \ldots \), when referring to a product state of triplets and singlets in left/right, valley and spin spaces.

As it is shown in detail in the next subsections, for cases A, B and C the sixteen \((1,1)\) eigenstates for zero hyperfine are associated with 3, 9 and 10 energy levels, respectively, that sometimes cross each other or become degenerated. These situations change drastically the outcome of the return probability experiment. In order to present the correspondence between the \((1,1)\) states and these energy levels, we divide the states into two classes. In the first class, as in Sec.II D, we take six groups, each one corresponding to a LR-even/LR-odd pair of states, i.e., \( |T^{LR}_{0}(n) \rangle \) and \( |S^{LR}_{0}(n) \rangle \). These six groups—that as shown in Table I, may belong to the same energy level—are of great importance for the return probability experiment because they are connected to the \((0,2)\) states, \( |T^{LR}_{0}(n) \rangle \), through the LR-even states. Apart from a global energy shift, these \((1,1)\) energy levels and each associated \((0,2)\) energy level have the same dependence with the parameters, therefore, we use the energy level labeling of Table I also for identifying the \((0,2)\) prepared states. The second class of states consists of the four fully polarized spin and valley LR-odd states, i.e., \( |S^{LR}_{\pm}(n) \rangle \); they belong to the energy levels listed in Table II. These blocked states do not provide access to the \((0,2)\) configuration neither at the preparation nor at the measurement stage, however, if their associated energy level crosses (or is degenerated with) an energy level with states of the first class, they become relevant for the effective hyperfine dynamics.

The labeling introduced in Tables I and II for the energy levels of case B and C—the less degenerated cases—is inspired by the following logic: “l”, “c” and “h” denote low, central and high, respectively, referring to the valley characters of the states associated with the energy level. Similarly, the +, − and 0 refer to the spin characters. Since two pairs of LR-partners states fall in level \( c_0 \), we distinguish them (in case C because \( \Delta_{so} \neq 0 \) splits the \( c_0 \) level) by adding the subscript “H” or “L” for the high and the low energy LR-partner states, respectively.

2. Labeling of the different physical situations

In what follows the numbers \( n_e \) and \( n_{(0,2)} \) are useful for distinguishing different qualitative and quantitative dynamical situations. For this reason, we label each case using the two integers as \( n_{en(0,2)} \). As an example, with the latter convention, the case in which the \((1,1)\) subspace is fully degenerated is to be labeled as “160” because \( n_e = 16 \) and \( n_{(0,2)} = 6 \); in such a case six independent prepared states provide access to the full subspace of evolution. As another example, a crossing between the energy levels \( c_{0L} \) and \( b_0 \) (presented in Table I) implies a subspace of evolution with \( n_e = 4 \) containing two LR-symmetric states (one associated with level \( c_{0L} \) and the other with level \( b_0 \)) that can be prepared, therefore, this situation is to be labeled as “42”.

However, as we show below, in some cases two situations with the same \( n_e \) and \( n_{(0,2)} \) numbers but different HFI dynamics appear; in such cases we use a superscript

---

### Table I. Energy levels and labels for the six LR-even/LR-odd partner states in the \((1,1)\) configuration for cases A, B and C.

| \( n,n' \) | Case A | Case B | Case C | Behavior |
|-----------|--------|--------|--------|-----------|
| \( K \uparrow, K \downarrow \) | \( v_0 \) | \( h_0 \) | \( h_0 \) | \( E_{orb} \) |
| \( K' \uparrow, K' \downarrow \) | \( v_0 \) | \( l_0 \) | \( l_0 \) | \(-E_{orb} \) |
| \( K \uparrow, K' \downarrow \) | \( v_0 \) | \( c_{0L} \) | \( c_{0L} \) | \(-\Delta_{so} \) |
| \( K \downarrow, K' \uparrow \) | \( v_0 \) | \( c_0 \) | \( c_0 \) | \( \Delta_{so} \) |
| \( K \uparrow, K' \downarrow \) | \( v_0 \) | \( c_+ \) | \( c_+ \) | \( E_{s} \) |
| \( K \downarrow, K' \uparrow \) | \( v_0 \) | \( c_- \) | \( c_- \) | \(-E_{s} \) |
The return probability is also given in the figure as tags to quantum numbers. Connected to their \((0,2)\) partners with same spin and valley such that only left/right symmetric \((1,1)\) states are connected. The connections of \((0,2)\) and \((1,1)\) singlet/triplet notation for spin, valley and left/right symmetric states in the evolution subspace, \(|T_{0}^{LR}S_{n,m}\rangle\), and its LR-antisymmetric partner state, \(|S_{LR}T_{n,n'}\rangle\).

**A. Case A: \(\Delta_{\text{so}}=0\) and \(E_{\text{orb}}=0\)**

The single-particle spectrum of a single dot (in the absence of HFI) is shown in Fig.2(a) as a function of the magnetic field. As shown in the legend, \(P_{g}\) is found to be 0.4, 0.50 or 3/8 depending on both the magnetic field value and the prepared \((0,2)\) state.

\(\text{“s” or “n” to distinguish them. The “n” superscript is reserved for cases in which the effective HFI Hamiltonian has a zero matrix element between any of the LR-symmetric states in the evolution subspace, } |T_{0}^{LR}S_{n,m}\rangle\text{, and its LR-antisymmetric partner state, } |S_{LR}T_{n,n'}\rangle.\)

**FIG. 4. Case A: Saturation return probabilities, energies and states for a valley degenerated DQD; \(\Delta_{\text{so}}=E_{\text{orb}}=0\) and the Zeeman splitting is \(E_{S}=g_{\mu}B.\) The associated single dot single-particle spectrum is shown in Fig.2(a). (Left panel) Eigenstates and spectrum of the \((0,2)\) and \((1,1)\) configurations; the degeneracy of each energy level at finite magnetic field is indicated. The six \((0,2)\) states in levels 0, 4, 8, 12, 16 and 20 are presented.

The right panel of Fig.4 shows the energies of the \((1,1)\) states by tunneling are shown with double headed arrows, to a single LR-symmetric state in \((1,1)\). (Right panel) Energy levels in the \((1,1)\) configuration as a function of the magnetic field; as shown in the legend, \(P_{g}\) is found to be 0.4, 0.50 or 3/8 depending on both the magnetic field value and the prepared \((0,2)\) state.

\(\text{The Case } 16_{0}\text{ (in Fig.4) is for zero magnetic field, leading to the largest possible degeneracy, } n_{v}=16. \text{ All the } (0,2)\text{ eigenstates are connected to this subspace and hence the state counting estimation for the saturation return probability is } P_{g}\text{, where the state counting gives 1/4, whereas coherent evolution gives return probability 1/3. Interestingly, in both cases one goes from } P_{g}\text{ to the correct result by subtracting 1 from the denominator, since 6/(16-1)=0.4.}\)

We have also studied the final state resolved saturation return probabilities and observed that it is not the same for the six \((0,2)\) states. It is more probable to return to the \((0,2)\) state that was prepared, and this is more pronounced when the prepared state is one of the two nonzero-spin states (the states \(T_{0}^{LR}S_{n,m}\)). In Fig.5(a) we show that the decaying time \(t_{d}\) (see Fig.1(b)) here depends on the prepared \((0,2)\) state, being longer for the nonzero-spin prepared states, 0.185\(/\sigma_{b}\text{, while for the remaining four prepared states it is 0.149}\text{. We discuss below, when introducing cases 8s}^{1}\text{ and 4p}^{1}, \text{the reason of such an asymmetry.}\)

It is worth to introduce here the structure of the hyperfine field interaction Hamiltonian, \(H_{h,LR}^{SP}\text{ using the sixteen } (1,1)\text{ basis states presented in Fig.4 and Tables I and II. In the octahedral representation given in Fig.5(c) each vertex stands for a LR-symmetric state and its LR-antisymmetric partner state. Therefore, the initial } (1,1)\text{ state at } t_{d} = 0 \text{ has weight in the LR-even states located on those six vertices. The links in solid lines between vertices and the links in dotted lines with the remaining LR-antisymmetric states represent nonzero matrix elements of the HFI. Each link stands for both homogeneous and inhomogeneous elements of the hyperfine field. The absence of matrix elements be-}
FIG. 5. Scheme of the complete hyperfine Hamiltonian (right panel) and the return probabilities $P(\tau_s)$ for case A (left panels), i.e., $\Delta_{\infty} = E_{\text{orb}} = 0$; see Fig.4. (a) Zero magnetic field, type $16_6$ dynamics, all prepared states give $P_\infty = 0.40$ but $P(\tau_s)$ decays faster for total spin zero prepared states. (b) Finite magnetic field. Type $8_3$ dynamics is found when a zero spin state is prepared, $P_\infty = 0.50$. For nonzero spin prepared states one has type $4^s$ dynamics and $P(\tau_s)$ follows Eq.(54) giving $P_\infty = 3/8$ (this situation also appears for the DQDs with $\Delta_{\infty} \neq 0$ of case C, see Fig.8). (c) Scheme of the full 16 by 16 HFI Hamiltonian, $H_{16}^{\text{LR}}$; we label the states according to the ten energy levels they belong in case C. The six octahedron’s vertices represent LR-odd/LR-even partner states of Table I; note that the HFI matrix element between these partners, $\Delta \equiv 0$, is zero for the $c_\pm$ and the $c_\mp$ vertices. Outside the octahedron the four LR-odd states of Table II are represented (for simplicity, only two are shown). The links between nodes represent the existence of at least one nonzero matrix element between the states. Depending on the parameters—for cases A, B and C—the ten energy levels ($c_\pm, c_{\pm h_0}, h_0, s, h_\pm, l_\pm$, and $l_\mp$) can move together and/or cross each other, leading to the eight different effective HFI dynamics involving less than sixteen $(1,1)$ states.

In Fig.5(c) we have used the labeling of the energy levels given in Table I for case C (see Fig.8), $c_\pm$, $c_{\pm h_0}$, $h_0$, $s$, $h_\pm$, $l_\pm$, and $l_\mp$. We show below that—depending on the parameters in cases A, B and C, as some of these ten energy levels move together and/or cross each other—there are eight different effective HFI dynamics involving restricted subspaces of evolution. For example, in the presence of spin-orbit coupling (case C below) the $16_6$ case becomes irrelevant because the hyperfine field (characterized by an energy scale, $\sigma_h$, which is smaller than $\Delta_{\infty}$) is unable to mix all the sixteen states and therefore the physical situation is better captured by analyzing smaller subspaces of evolution depending on the prepared state.

The Case $8_3$. A finite Zeeman energy is applied much larger than $\sigma_h$. The initialized $(0,2)$ state has zero spin and therefore belongs to the energy level $v_0$ with degeneracy $n_{(0,2)} = 4$. The corresponding $(1,1)$ subspace in which the system evolves has a degeneracy of $n_e = 8$, with four LR-symmetric states. In this case, the state counting estimation for the saturation return probability, being $P_{\infty}^{8_3} = 4/8 = 0.5$, coincides with the calculated exact result. Moreover, as shown in Fig.5(b), the values of $P_\infty$ and the shape of $P(\tau_s)$ do not depend on which of the four $(0,2)$ states is being prepared. Finally, we find that the decaying time, here $\tau_s \approx 0.238h/\sigma_h$, is larger than both possible decay times for the zero-field case, which is expected because for the $16_6$ case the HFI has the ability to mix the prepared state with eight extra states.

The independence on the prepared state can be understood from the matrix elements of the Hamiltonian in the reduced Hilbert space by using the singlet/triplet functions. The HFI term proportional to $\delta h_z(0)$ mixes only by one the four zero-spin pairs of LR-symmetric and LR-antisymmetric states as follows:

$$\langle S_{LR}^{T \pm}, K, \kappa' | H_{LR}^{2p} | S_{LR}^{T \pm}, K, \kappa' \rangle = 2\delta h_z(0).$$

The fact that the subspace $c^{8_3}$ is composed solely by LR-symmetric states and their LR-antisymmetric partners is a key difference to the other cases where the state counting argument fails, because in those cases more states are available.

An illustration of all the matrix elements $H_{LR}^{8_3}$ can be
extracted from the full Hamiltonian representation in Fig.5(c), by considering solely the four octahedron vertices in the plane (because the \( v_0 \) level contains all the states in nodes \( b_0, b_0' \) and \( c_0 \)) and excluding the \( c_+ \) and \( c_- \) vertices. In accordance with Eq.(49), the HFI matrix element between the included LR-partners, \( m \) in the figure, is nonzero. The remaining matrix elements (links in the figure) connect each LR-symmetric state with other two LR-symmetric states and their LR-antisymmetric partners. All those matrix elements follow Gaussian distributions with the same variance and thus, the average result is independent of which \( T_{LR}^n \) state is initialized. This symmetry is also responsible for the distribution of the total saturation probability (1/2) evenly among the four \( T_{LR}^1 \) states.

The case \( 4^{1}_+ \) (Fig.4) is also for \( E_s \geq \sigma_h \) but here the initial state belongs either to the energy level \( v_+ \) or the \( v_- \).

In Sec.IV C the same situation is found for a particular value of the parallel magnetic field in a nanotube with \( \Delta_{\text{ez}} \neq 0 \). Here we present an analytical derivation of the return probability in the reduced Hilbert space, which we have also confirmed by a full numerical evaluation. We find that the saturation return probability is

\[
P_s^{4^{1}_+} = 3/8 = 0.375.
\]

We restrict the analysis to the states of the energy level \( v_+ \), and equivalent results for level \( v_- \) follow by symmetry. The system is prepared in the \( T_{LR}^1 \) state and after separation the initial (1,1) state is initialized. This symmetry is also responsible for the distribution of the total saturation probability (1/2) evenly among the four \( T_{LR}^1 \) states.

\[
\frac{1}{2} = \frac{1}{4} (1,1) + \frac{1}{4} (2,2).
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The energy level \( v_+ \) (1,1) is the 4-dimensions identity matrix and \( \sigma_h \) is the 4-dimensions antisymmetry matrix. The system is prepared in the \( T_{LR}^1 \) state and after separation the initial (1,1) state is initialized. This symmetry is also responsible for the distribution of the total saturation probability (1/2) evenly among the four \( T_{LR}^1 \) states.

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\[
\frac{1}{2} = \frac{1}{4} (1,1) + \frac{1}{4} (2,2).
\]
present the spectrum for the (0,2) and (1,1) configurations including the level degeneracies at finite magnetic field and the corresponding states. In the figure, we take a ratio $E_{orb}/E_s=2g_{orb}/g_s$ $\phi$ bigger than one; which is the typical case for fully parallel magnetic field. The five energy levels of the (0,2) configuration $e_{\pm}$, $c_0$, $l_0$ and $h_0$—follow from Eq.(23) and are given in Tables I and II.

For zero field all the degeneracies remain and the situation reduces to the $16_0$ case already analyzed in Sec.IVA. At finite $B||$, the return probability experiment can have two different behaviors as indicated in the right panel of Fig.6. When one of the four spin-zero states is prepared, we get $P_{20}^T=2^1/2$, whereas a nonzero spin prepared state is unaffected by the hyperfine interaction and thus $P_{20}^T(\tau_s)=1$. We explain these two cases in the next paragraphs.

In the case labeled $2^1$ the initial state belongs to the $h_0$, $l_0$ or to the $c_0$ energy levels. The degeneracy for the (1,1) states in $l_0$ or in $h_0$ is 2, and $n_{(0,2)}=1$, in each case corresponding to a pair of LR symmetric/anti-symmetric states. On the other hand the $c_0$ level has a 4-fold degeneracy and two LR-even states are connected to (0,2); however, the structure of the hyperfine interaction Hamiltonian allows us to treat the subsets of double degenerated states, $c_{0L}$ and $c_{0H}$ presented in Table I, as two independent pairs with $n_c=2$ and $n_{(0,2)}=1$. This follows from the selection rule introduced above when explaining the absence of matrix elements for states at opposite vertices of the octahedron in Fig.5(c).

Here the state counting prediction for the saturation return probability (being $P_{20}^T=2^1/2$) coincides with the exact result. The $2 \times 2$ effective Hamiltonian that describes the four cases follows from Eq.(49) and it is given by

$$H_{e}^2 = \begin{pmatrix} 0 & 2\delta h_z^{(0)} \\ 2\delta h_z^{(0)} & 0 \end{pmatrix}. \quad (56)$$

In Appendix A we derive that the return probability is

$$P_{20}^T(\tau_s) = \frac{1}{2} + e^{-8(\sigma_s \tau_s / h)^2} \frac{1}{2}, \quad (57)$$

which is shown in Fig.7. From Eq.(43) one readily obtains $\tau_d = \sqrt{\frac{\ln 2}{\delta h_z^{(0)}}} h / \sigma_h \approx 0.2944 h / \sigma_h$.

FIG. 7. Return probabilities $P(\tau_s)$ for case B, i.e., zero spin-orbit coupling but coexistence of Zeeman and orbital effects due to the parallel component of the magnetic field (see labels in Fig.6). Depending on the prepared state the return probability have two behaviors: (i) type $2^1$ —with $P_{20}^T=1$—when one of the two nonzero-spin states are prepared or (ii) type $4_0^1$ —with $P_{20}^T=1/2$; see Eq.(57)—when one of the remaining four states is prepared.
FIG. 8. Case C: Saturation return probabilities, energies and states for a nanotube-based DQD with spin-orbit coupling in a parallel magnetic field, i.e., \( \Delta_{so} \neq 0 \), \( E_{orb} \neq 0 \) and \( E_z \neq 0 \); the single dot single-particle spectrum is shown in Fig.2(c) (Left panel) Scheme of the (0,2) and (1,1) energy levels and the associated states; the level degeneracies for finite magnetic field are indicated. Each one of the six (0,2) states is connected by inter-dot tunneling to a single associated (1,1) state. For the (1,1) charge state the LR-symmetric and LR-antisymmetric states are distinguished. (Right panel) Energy levels in the (1,1) configuration as a function of the magnetic field; dashed levels contain only blocked states and therefore cannot be prepared. As shown in the legend—for the fifteen level crossings at \( B_n \), with \( i = 0, \ldots, 8 \) and the six generic situations at any non-crossing field, \( B_{nc} \)—the return probability presents seven different types of dynamics and \( P_{2i}^c \) is found to be 1/3, 3/8, 1/2 or 1 depending on both the magnetic field value and the prepared (0,2) state.

This type of dynamics is equivalent to the situation for a GaAs double dot in large Zeeman field, in which case only the spin triplet \( S^{LR,T}_{0} \) and the spin singlet \( T^{LR,S}_{0} \) are—neglecting tunneling exchange—degenerated: in the system the \( z \)-component of the hyperfine field (see Eq.(39c)) is responsible for the mixing of these two states.\(^{11,18,20} \) In the present case an equivalent physical situation is realized for four out of the six possible prepared (0,2) states.

**In the case** \( 2E_{\parallel} \) the prepared state belongs to one of the two (0,2) energy levels \( c_n \) and \( c_{-n} \), where the states are the spin-polarized valley singlets:

\[
T^{LR,S}_{0} \text{val}_{s_n} \text{spin} \text{in level} \ c_{s_n}, \ \text{with} \ s_n = \pm.
\]  
(58)

After separation the system is initialized at the associated LR-even state, \( T^{LR,S}_{0} \text{val}_{s_n} \text{spin} \), which is degenerated with its LR-odd partner, \( S^{LR,T}_{0} \text{val}_{s_n} \text{spin} \). As shown previously (see Eq.(53)), the hyperfine interaction does not have matrix elements between these two states. The return probability is therefore \( \tau_\pm \)-independent and equal to one

\[
P_{2i}^c (\tau_\pm) = 1.
\]  
(59)

This somewhat counterintuitive result has been reported previously in Ref. 24, where the same saturation value is found in silicon double dots—taking into account a valley conserving HFI—for some particular prepared states that, as here, the hyperfine field is unable to mix with other states.

**C. Case C: \( \Delta_{so} \neq 0 \) and \( E_{orb} \neq 0 \)**

Here we consider a double dot based on the single dot presented in Fig.2(c). Figure 8 shows the energy levels and states of the (0,2) and (1,1) configurations, which follow from Eqs.(12) and (13). The right panel depicts the ten levels of the (1,1) spectrum as a function of the total magnetic field which is parallel to the tube axis. In the figure, we use solid lines for the six energy levels having LR-even states, those states are accessible from (0,2). By preparing a state in those levels the return probability experiment can be performed; at the evolution stage, it becomes accessible to the HFI each and every state belonging to others energy levels if they are degenerated with the energy level that holds the prepared state and, therefore, level crossings must be studied. As it is shown in Fig.8, it is intrinsic to this case the existence of level crossings for zero magnetic field and also at finite values of the magnetic field. Finite magnetic field crossings (involving at least one energy level with a LR-even state) occur at

\[
B_1 = \frac{\Delta_{so}}{\mu_B (4g_{orb} + g_s)}, \quad B_2 = \frac{\Delta_{so}}{\mu_B (4g_{orb} + g_s)}, \quad B_3 = \frac{\Delta_{so}}{\mu_B (2g_{orb} + g_s)} ,
\]  
(60a)

\[
B_4 = \frac{\Delta_{so}}{2\mu_B g_{orb}}, \quad B_5 = \frac{\Delta_{so}}{\mu_B (2g_{orb} - 2g_s)}.
\]  
(60b)

\[
B_6 = \frac{\Delta_{so}}{\mu_B (2g_{orb} - 2g_s)}.
\]  
(60c)
\[ B_7 = \frac{\Delta_{\sigma_0}}{\mu B (2g_{\text{orb}} - g_\gamma)} , \quad B_8 = \frac{\Delta_{\sigma_0}}{\mu B g_\gamma} , \quad (60d) \]

the \( B_7 \) and \( B_8 \) of Eq. (60) being positive values of the magnetic field given that we have assumed \( E_{\text{orb}} > E_s \) and therefore \( 2g_{\text{orb}} > g_\gamma \). We identify twenty-one different situations, the six non-crossing cases and the fifteen level crossings. In the right panel of Fig.8 we label each case according to its type of dynamics and we give the value of \( P_\infty \) in the legend. We describe all those situations below.

1. Zero magnetic field

As shown in Fig.2(c) in the single-particle description, the spin-orbit coupling breaks the 4-fold degeneracy resulting in two Kramers doublets; the lowest energy Kramers doublet in the quantum dot \( \xi \geq (L \text{ or } R) \) consists of the pair of time-reversal states \( |\xi K \uparrow \rangle \) and \( |\xi K' \downarrow \rangle \), whereas the highest energy Kramers doublet groups the states \( |\xi K' \uparrow \rangle \) and \( |\xi K \downarrow \rangle \). With double occupation of the right dot—states and levels shown in Fig.8—for the state at level \( c_{0L} \) (\( c_{0H} \)) the two electrons occupy the lowest (highest) energy Kramers doublet in dot configuring the non-degenerated ground (highest excited) state of the (0,2) configuration. Right at the middle energy between the last two states the levels \( c_+ \), \( c_- \), \( l_0 \) and \( h_0 \) are degenerated: they correspond to the four (0,2) states with one electron in each of the Kramers doublets.

For the type 4^1 \( _s \) presented in Fig.8 the return probability behaves identically when the prepared state is the (0,2) ground state (level \( c_{0L} \) identified below by \( \sigma = + \)) or the (0,2) highest exited state (level \( c_{0H} \) identified below by \( \sigma = - \)). After separation the LR-even state becomes a member of an (1,1) evolution subspace with \( n_c = 4 \), the four states are

\[ |1, 4^1 _s, \sigma \rangle = T_0^{LR} S_{K; \sigma; \tau} , \quad |2, 4^1 _s, \sigma \rangle = S^L R^{T_{K; \sigma; \tau}} , \quad |3, 4^1 _s, \sigma \rangle = S^L R^{T_{\text{val}}^{\uparrow \downarrow} \epsilon_{\tau}} , \quad |4, 4^1 _s, \sigma \rangle = S^L R^{T_{\text{val}}^{\downarrow \uparrow} \epsilon_{\tau}} , \quad (61) \]

where in the spin triplets the subindex \( \sigma \) is to be interpreted as + or - instead of \( \uparrow \) or \( \downarrow \) respectively. In this space the effective Hamiltonian \( H_{\text{eff}}^{4^1 _s} \) is analogous to a double dot in GaAs described by the Hamiltonian in Eq.(51). The equivalence with the components of the hyperfine field given in Eq.(38) is as follows

\[
\begin{align*}
\delta h_x &\rightarrow \sigma \delta h_z^{(0)} , \\
\delta h_y &\rightarrow \sigma \delta h_z^{(0)} , \\
\delta h_z &\rightarrow \sigma \delta h_y^{(0)} , \\
\delta h_{x'} &\rightarrow \delta h_z^{(1)} , \\
\delta h_{x''} &\rightarrow \delta h_z^{(1)} , \\
\delta h_{y'} &\rightarrow \delta h_z^{(2)} , \\
\delta h_{y''} &\rightarrow \delta h_z^{(2)} .
\end{align*}
\]

(62a)

(62b)

From Eq.(30) we obtain that the components of the effective hyperfine field

\[ h_j^L = \bar{h}_j + \delta h_j , \quad h_j^R = \bar{h}_j - \delta h_j \quad \text{for } j = x, y, z , \quad (63) \]

follow Gaussian distributions with identical standard deviations \( \sigma_{\delta h} = \sqrt{2} \sigma_{\delta h} \). Therefore, the situation is mapped exactly to a spin-only double dot at zero field and the return probability is then

\[ P_{\text{eff}}^{4^1 _s} (\tau_s) = \frac{1}{3} (1 + g (\tau_s, \sigma_{\delta h} / \hbar) + g^2 (\tau_s, \sigma_{\delta h} / \hbar)) , \quad (64) \]

where \( g(x) \equiv e^{-2x^2} (1 - 4x^2) \). A derivation of this result is presented in Appendix A. This well-known shape, shown in Fig.9(a), leads to \( P_{\infty}^{4^1 _s} = 1/3 \) and so the state counting estimation, which is this case is 1/4, fails. Finally, for this shape the decaying time defined in Eq.(43) is \( \tau_s \approx 0.18935 \hbar / \sigma_h \).

In the case \( \xi \) the prepared (0,2) state belong to the energy level \( c_+ \), \( c_- \), \( h_0 \) or \( l_0 \). At \( B_0 = 0 \) the four levels have the same energy and therefore, after the separation stage, the evolution subspace in (1,1) includes their four LR-even partners and the associated LR-odd states, i.e., \( n_c = 8 \). For all these prepared states we find \( P_{\infty}^{4^1 _s} = 0.50 \), but the shape of \( P_{\text{eff}}^{4^1 _s} (\tau_s) \), shown in Fig.9(a), depends on the prepared state. The decaying time is \( \tau_s \approx 0.301 h / \sigma_h \) when the prepared state belongs to the level \( c_+ \) or \( c_- \) and \( \tau_s \approx 0.201 h / \sigma_h \) when the prepared state belongs to the level \( h_0 \) or \( l_0 \). From the full HFI Hamiltonian in Fig.5(c) one can visualize the Hamiltonian of the hyperfine field for this subspace, \( H_{\text{eff}}^{4^1 _s} \), by considering states at the octahedron vertices excluding \( c_{0L} \) and \( c_{0H} \) vertices. The difference in the decaying times arises because, as shown in Eq.(53), there are no direct matrix elements of the HFI Hamiltonian between the nonzero-spin LR-even/LR-odd partners; i.e., \( m = 0 \) for \( c_+ \) and \( c_- \) in Fig.5(c).

2. Finite magnetic field

There is a set of situations—including any non-crossing of the magnetic field, \( B_{nc} \)—in which the return probability is analogous to the cases without spin-orbit coupling introduced in Sec.IV.B. This happens for the following situations (see crossings at Fig.8):

(i) When the prepared state belongs to the energy level \( l_0 \) at \( B_1 \) (or \( h_0 \) at \( B_2 \)) because \( T_{\text{val}}^{\uparrow \downarrow} \) and \( T_{\text{val}}^{\downarrow \uparrow} \) are not mixed by the HFI. The return probability is type \( 2^1 _s (P_{\infty} = 1/2) \).

(ii) When the prepared state belongs to the energy level \( c_- \) at \( B_3 \) (or \( B_0 \)) because \( T_{\text{spin}}^{\uparrow \downarrow} \) and \( T_{\text{spin}}^{\downarrow \uparrow} \) are not mixed by the HFI. The return probability is type \( 2^1 _s (P_{\infty} = 1) \).

(iii) When the prepared state belongs either to the energy level \( c_{0H} \) (one electron in \( K \downarrow \)) and the other in \( K' \uparrow \)) at \( B_3 \) or, to level \( c_{0L} \) (one electron in \( K' \downarrow \)) and the other in \( K' \uparrow \)) at \( B_7 \). At \( B_3 \), the level \( c_{0H} \) crosses \( h_+ \) (both electrons at the \( K' \downarrow \) state) and, at \( B_7 \), the level \( c_{0L} \) crosses \( l_+ \) (both electrons at the \( K' \uparrow \) state). The hyperfine field does not introduce mixing at these two crossings because in each one of them the LR-odd state have
FIG. 9. Return probabilities \( P(\tau_s) \) that appear only for case \( C \), i.e., \( \Delta_{so} \neq 0 \) in a parallel magnetic field. (a) At zero field one gets \( P_s = 1/3 \) (type 4\( _1 \)) or \( P_s = 1/2 \) (type 8\( _1 \)). In the latter case the probability decays slower if the prepared state is a spin polarized valley singlet. (b) All cases give \( P_s = 1/2 \) for type 4\( _1 \) presented in panel (a).

### Table: Prepared states

| Type | Prepared state |
|------|----------------|
| 4\(_1\) | \( c_{0a}, c_{0b} \) \( h_0, h_0 \) \( P_s = 0.50 \) |
| 8\(_1\) | \( c_{0a}, c_{0b} \) for \( B_4 \) \( c_{0a}, c_{0b} \) for \( B_8 \) |

**D. Case D: \( \Delta_{so} \neq 0 \) and \( B_\perp \neq 0 \)**

Here, in contrast to cases A, B and C, the spin projection along the direction of the magnetic field is not a good quantum number. The perpendicularch field, \( B_\perp \), introduces a Zeeman energy \( E_z = g\mu_B B_\perp \) and zero diamagnetic effects. Due to the competition between the Zeeman interaction and the spin-orbit coupling the single-particle and single dot problem has eigenstates with spin projection in the plane generated by the tube axis and the direction of the magnetic field. In the following the tube axis is chosen along the \( z \)-direction and the magnetic field is applied along the \( x \)-direction. The solutions are

\[
\begin{align*}
|K, +\rangle &= |K\rangle \otimes \left( \cos \frac{\eta}{2} |\downarrow\rangle + \sin \frac{\eta}{2} |\uparrow\rangle \right), \\
|K', +\rangle &= |K'\rangle \otimes \left( \cos \frac{\eta}{2} |\uparrow\rangle + \sin \frac{\eta}{2} |\downarrow\rangle \right), \\
|K, -\rangle &= |K\rangle \otimes \left( \cos \frac{\eta}{2} |\uparrow\rangle - \sin \frac{\eta}{2} |\downarrow\rangle \right), \\
|K', -\rangle &= |K'\rangle \otimes \left( \cos \frac{\eta}{2} |\downarrow\rangle - \sin \frac{\eta}{2} |\uparrow\rangle \right),
\end{align*}
\]

where \( \eta \equiv \arctan E_z/\Delta_{so} \). The eigenenergies \( E_{\pm} = \pm \frac{1}{2} \sqrt{\Delta_{so}^2 + E_z^2} \) are shown in Fig.2(d). From hereon we use the doublet index, \( d = \pm \), to identify the two doublets. The tunneling Hamiltonian is still diagonal in this

\[
\delta h_j \mapsto \delta h_{j,0}, \quad \tilde{h}_j \mapsto \tilde{h}_{j,0} \quad \text{for } j = x, y, z.
\]
basis, which means that each (0, 2) state mixes with only one (1, 1) state and the tunneling energy gap is \( \Delta = 2\sqrt{2}t \), as before.

We now show that the perpendicular field situation reduces to a modified version of cases already considered in the paper. When the single-particle states are well separated on the scale of the HFI only the matrix elements of the HFI Hamiltonian between the \( d = + \) solutions or in between the \( d = - \) solutions enter. The result falls in between the \( 2 \times 2 \) effective hyperfine field for the dot \( \xi \) and the doublet \( d \) can be writing as

\[
H^{\xi,d}_h = (h^{\xi,d}_{0,0} + h^{\xi,d}_{x,2} \sigma_x^d + h^{\xi,d}_{y,2} \sigma_y^d + h^{\xi,d}_{z,2} \sigma_z^d),
\]
where \( \xi = L, R \) and \( \sigma_j^{\xi,d} \) are Pauli and identity matrices in the doublet space. The coefficients are given by

\[
\begin{align}
    h^{\xi,d}_{0,0} &= h^{(0)}_{x \xi} d \sin \eta, \\
    h^{\xi,d}_{x,2} &= h^{(1)}_{x \xi} + h^{(2)}_{y z} d \cos \eta, \\
    h^{\xi,d}_{y,2} &= h^{(2)}_{x z} - h^{(1)}_{y z} d \cos \eta, \\
    h^{\xi,d}_{z,2} &= -h^{(0)}_{x \xi} d \cos \eta.
\end{align}
\]

The Hamiltonian \( H^{\xi,d}_h \) is equivalent to a spin in a Zeeman field, plus an energy shift, \( h^{\xi,d}_{0,0} \), which is irrelevant for the dynamics of the 2-level system. The values of the effective field components depend on the angle \( \eta \), i.e., on the external perpendicular magnetic field. Using the variances of the hyperfine components \( h^{(i)}_{j \xi} \) (for \( j = x, y, z \) and \( i = 0, 1, 2 \)) given in Eq.(30), it follows that the variances of the effective components in \( H^{\xi,d}_h \) are:

\[
\begin{align}
    \tilde{\sigma}_2^2 &= \left\langle \left( h^{\xi,d}_{x,2} \right)^2 \right\rangle = \left\langle \left( h^{\xi,d}_{y,2} \right)^2 \right\rangle = \sigma^2_2 (1 + \cos^2 \eta), \\
    \tilde{\sigma}_1^2 &= \left\langle \left( h^{\xi,d}_{z,2} \right)^2 \right\rangle = 2\sigma_2^2 \cos^2 \eta.
\end{align}
\]

The situation of the return probability behaves as situations already investigated:

(a) When \( E_s = 0 \) (i.e., \( \eta = 0 \)) the results are presented in Sec.IV.C for \( B_{\parallel} = 0 \).

(b) When \( E_s \gg \Delta_{\text{so}} \) (i.e., \( \eta \to \pi/2 \)) the behavior is as the situation presented in Sec.IV.A for nonzero magnetic field.

Away from these two limits, for any of the four (0, 2) prepared states having one electron in each doublet (\( R, + \) and \( R, - \)), the return probability goes smoothly from type \( S^0_1 \) (at \( E_s = 0 \)) to type \( S^0_2 \) (at \( E_s \gg \Delta_{\text{so}} \)). The situation is not so interesting since the saturation value \( P_{\infty} \) is always 0.50. The shape of \( P(\tau_d) \) and the decaying times \( \tau_d \) for each prepared state depend on the effective 8 \( \times \) 8 evolving (1,1) Hamiltonian. The result falls in between the two above mentioned limits (a) and (b). As shown in the previous sections the Hamiltonian for \( E_s = 0 \) is non-symmetric, while it is symmetric for \( E_s \gg \Delta_{\text{so}} \). In the latter case, \( P(\tau_d) \) is independent of the prepared state and a smaller decaying time is observed.

On the other hand, the value of the saturation return probability changes if the (0,2) ground state or the (0,2) highest excited state is prepared. The ground state is the following Slater determinant:

\[
\left| \Psi_{(0,2)}^{(s)}(\eta) \rightangle = \begin{cases} R_{K'}^{\text{LR}} & \\
R_{K}^{\text{LR}} & \end{cases} \left| T^{\text{LR}}_{\text{val}} S^{\text{LR}}_{\text{spin}} \rightangle
\]

At zero-field \( \eta = 0 \) and the prepared state is \( T^{\text{LR}}_{\text{val}} S^{\text{LR}}_{\text{spin}} \), and we find type \( 4^s \) behavior with \( P_{\infty} = 1/3 \). For a dominant Zeeman energy \( \eta = \pi/2 \) and the prepared state is the spin polarized valley singlet, \( T^{\text{LR}}_{\text{val}} S^{\text{LR}}_{\text{spin}} \), with the spin triplet along the \( x \)-direction; we then find type \( 4^s \) behavior with \( P_{\infty} = 3/8 \).

For the intermediate magnetic field regime, with the (0,2) state having two electrons in one doublet, the problem is mapped to a double dot without the valley degree of freedom in a hyperfine field with the variances of Eq.(69b). Following Appendix A, we obtain the return probability by computing the averages of Eq.(A10) with the probability distribution of Eq.(A11) providing that \( \sigma_{n_\parallel} = \sigma_{n_\perp} = \sigma_{\parallel} \) and \( \sigma_{n_\perp} = \sigma_{\perp} \).

We plot the standard deviations \( \tilde{\sigma}_\perp \) and \( \tilde{\sigma}_\parallel \) in Fig.10(a) as a function of \( E_s/\Delta_{\text{so}} \). There is an overall reduction of the HFI when the magnetic field increases, which explains the larger decaying time \( \tau_d \) plotted in Fig.10(b). Moreover, the standard deviation of the perpendicular component goes to zero, and in this limit the HFI becomes 2-dimensional, approaching type \( 4^s \) behavior. Thus, the
initial state in Eq.(70) becomes a valley singlet and the hyperfine interaction is unable to mix directly with the $T_0$ partner. The saturation value of the return probability is presented in Fig.10(b). $P_\infty$ can take any value between 1/3 and 3/8 as a function of the magnetic field. This interesting result allows a direct measurement of the spin-orbit coupling splitting and the hyperfine intervalley mixing (see $x$ and $y$-components of the effective HFI in Eq.(68)) and its relation with the valley conserving hyperfine mixing ($z$-component of the effective HFI).

V. CONCLUSIONS

We have analyzed the expected return probabilities for a dephasing measurement in clean carbon nanotube based double quantum dots. We have focused on the intrinsic properties and therefore neglected disorder induced valley mixing and also Coulomb exchange, which are predicted and measured to be small in multi-electron dots. In a forthcoming publication, we study the influence of valley mixing.

We have shown that a multiple number of scenarios exists for the return probability experiment, due to the valley degree of freedom (as in Si-based DQDs) which makes the system very different from a double dot in a 2-dimensional electron gas (2DEG). Here, more specifically, these scenarios are due to: (i) the non-trivial structure of the hyperfine coupling with the $^{13}$C nuclei that affects both the electron spin and valley degrees of freedom; (ii) the experimental preparation protocol that determines which of the six (0,2) states is prepared; (iii) the availability of sixteen (1,1) states for the system in the evolution stage; (iv) the change (for every possible prepared state) of the subset of (1,1) states accessible in the evolution stage, and (v) the manifold of six possible return (0,2) states. The last point is an important difference to the 2DEG-based double dots, where only spin singlet returns to (0,2). Here the projection onto (0,2) is more generally determined by symmetry of the wavefunction, allowing only even left-right components to return. The level structure of the sixteen (1,1) and six (0,2) states depends on the values of the spin-orbit coupling and of the external magnetic field, through the Zeeman interaction, diamagnetic effects, or both.

In a 2DEG-based double dot the return probability shows two different behaviors being, type 4 dynamics ($P_\infty = 1/3$) for zero field, or, type 2 dynamics ($P_\infty = 1/2$) in the high magnetic field limit (we use the labeling introduced in Sec.IV). Here, depending on the parameters we find seven additional types of dynamics leading to saturation values $P_\infty = 3/8, 0, 1/2$ and 1. The results for all the nine situations are presented in Table III.

Type 16$_n$ dynamics can be found for zero magnetic field in the absence of spin-orbit coupling. In the cases with $\Delta_{\sigma o} = 0$, the behavior of a Zeeman interaction only system (type 8$_n$ and 4$_n$) is very different from the situation with both Zeeman and diamagnetic effects (type 2$_1$ and 2$_n$). For nonzero spin-orbit, the breaking of the spin degeneracy replaces, for zero magnetic field, type 16$_n$ behavior with type 8$_n$ and the well known type 4$_n$. At finite magnetic fields (when considering both Zeeman and diamagnetic effects) situations 2$_1$, 2$_n$, 4$_2$, 4$_n$, 4$_n$ and once again 4$_n$ can be obtained depending on the value of the magnetic field and on the prepared state.

In only two out of these seven novel situations (types 2$_0$ and 4$_0$), the return probability is associated with the system returning to the original prepared (0,2) state (see point (v) above). In all the remaining cases the system can be measured and also prepared in more than one (0,2) state, and therefore the functional dependence of the return probability on $\tau$ depends on both the prepared state and the dynamics type. We have defined a shape-independent decaying time and we find, $\tau_d \approx 0.149\sigma_h$, in the fastest case (for zero spin prepared states in type 16$_n$ dynamics) and an infinite decaying time (since the system does not decay for type 2$_n$ dynamics) in the slowest case. It should be noted that we have assumed throughout that the time scale of the experiment is much smaller than $T_1$, the inelastic dephasing time; otherwise inelastic processes would relax the system to the ground state invalidating the investigation of the dephasing in the return probability experiment as purely due to the hyperfine interaction. Therefore, the transient that defines the decaying time presented in Table III, $\tau_d$, is to be understood as valid only for evolving times, $\tau_s$, smaller than $T_1$.

In addition to the robustness of case 2$_n$ we find, for types 16$_n$, 8$_n$, 4$_2$, 4$_n$, asymmetries and/or long decaying times if the prepared state is a spin polarized valley singlet. The reason is that the hyperfine coupling of Eq.(36) does not introduces direct matrix elements between the LR-even spin polarized valley singlets and their LR-odd partners (see Eq.(53)); these two states can only be mixed by an inhomogeneous (in LR space) time-reversal symmetric term (i.e., spin-orbit coupling like), which does not appear in the HFI. In Ref. 26 it has been shown that this intrinsically anisotropic hyperfine field gives rise to a dip in the spin-blockade signal as a function of the orbital field.

Here, we have shown that this property of the hyperfine

| $P_\infty$ | Type | Cases | $r_{\sigma o}/\hbar$ | $r_{\sigma o}/\hbar$ |
|----------|------|-------|---------------------|---------------------|
| 1/3 | 4$_1$ | C | 4 | 1 | \(\approx 0.19935\) |
| 3/8 | 4$_1$ | A and C, B = 0 | 4 | 1 | 0.3218 |
| 0.40 | 16$_n$ | A and B, B = 0 | 16 | 6 | 0.185 | 0.149 |
| 1/2 | 2$_1$ | B and C, B = 0 | 2 | 1 | - | 0.2944 |
| 0.5 | 8$_1$ | A | 8 | 4 | 0 | -0.238 |
| 0.5 | 8$_n$ | C, B = 0 | 8 | 4 | 0.3014 | 0.2011 |
| 0.5 | 4$_2$ | C, B = B$_4$ | 4 | 2 | - | 0.2655 |
| 0.5 | 4$_2$ | C, B = B$_4$ | 4 | 2 | 0.4366 | 0.2327 |
| 1 | 2$_n$ | B and C, B = 0 | 2 | 1 | - | - |
field also leads to an interesting behavior of the return probability when the (0, 2) ground (or the highest excited) state is prepared for the case with nonzero spin-orbit coupling and the magnetic field is perpendicular to the tube axis, \( B_{\perp} \). As a function of the Zeeman energy, \( E_z \), the groundstate changes from a spin-unpolarized state (for \( E_z = 0 \)) to a spin-polarized valley singlet (for \( E_z / \Delta_{so} \gg 1 \)) and the saturation return probability goes from 1/3 (type 4\text{I}, i.e., effective 3-dimensional HFI) to 3/8 (type 4\text{II}, i.e., effective 2-dimensional HFI in the valley double dot). Measurement of \( P_{\infty} \) and \( \tau_d \) as a function of \( B_{\perp} \) would test the validity of the hyperfine Hamiltonian in Eq.(36) allowing, in principle, for the determination of the spin-orbit coupling and the hyperfine strength \( \sigma_h \).

Only a single return probability experiment\(^6\) has been reported in a carbon-based double dot. The result, only available for zero magnetic field, was an unexpected small return probability \( P_{\infty} \approx 1/6 \), that cannot be explained within the model presented here. We have shown that the minimum saturation return probability for coherent mixing is 1/3, similar to the situation in a spin-only double dot. Incoherent mixing will also not explain the experimental findings, since there the minimum return probability is 1/4, which could happen for crossings type 4\text{I} or 4\text{II}. We also note that by having worked in the high detuning limit in which the tunneling exchange is negligible we have obtained lower bounds of \( P_{\infty} \), since it is known that this coupling reduces the effectiveness of the hyperfine mixing and thus increases \( P_{\infty} \). One could speculate that valley mixing is responsible for the discrepancy. In a forthcoming publication, we discuss the role of such mixing, which however also cannot explain the small ratio between \( P(0) \) and \( P_{\infty} \) seen in experiment.

Clearly more experimental work is needed to better understand the rather rich structure of the carbon based double dots system, including the dependence of \( P(\tau_s) \) on magnetic field. One interesting aspect would be to design alternative preparation protocols for being able to select different initial (0, 2) states.

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Appendix A: Analytical calculation of \( P(\tau_s) \)

1. Mixing of a \( T^L_{LR} \), \( S^L_{LR} \) pair

This case (type 2\text{I} in Sec.IV) is valid whenever a LR-symmetric state and its partner LR-antisymmetric are mixed by the hyperfine interaction and no other states are involved the evolution Hamiltonian \( H_e \). In such a case the dynamics in the evolution subspace \( S_e \) is governed by the simple Hamiltonian:

\[
H_e^{2\text{I}} = \begin{pmatrix} 0 & 2\delta h_z^{(0)} \\ 2\delta h_z^{(0)} & 0 \end{pmatrix}.
\]

This Hamiltonian is valid for four out of the six \( T^L_{LR} \), \( S^L_{LR} \) pairs, specifically the zero-spin cases (see Eq.(49) and Eq.(53)). Here we use the notation of Eq.(25) and Eq.(20) for two single-particle single dot eigenstates with quantum numbers \( n \) and \( n' \) (\( n \) and \( n' \) must correspond to solutions with opposite spin projections).

Following Eq.(28) for \( \tau_s = 0 \) the state \( \text{LR}_{n,n'}^{even} \) is initialized. The system evolves as,

\[
\begin{align*}
|e(\tau_s)\rangle &= \cos \left( \frac{2\delta h_z^{(0)} \tau_s}{\hbar} \right) |\text{LR}_{n,n'}^{even}\rangle \\
&\quad + \sin \left( \frac{2\delta h_z^{(0)} \tau_s}{\hbar} \right) |\text{LR}_{odd}^{even}\rangle.
\end{align*}
\]

Therefore, for the realization \( r_i \) of the hyperfine field, the probability to find the system in the LR-even combination (i.e., to measure an (0, 2) charge state after the adiabatical joining stage) is just:

\[
P_r^{2\text{I}}(\tau_s) = \cos^2 \left( \frac{2\delta h_z^{(0)} \tau_s}{\hbar} \right).
\]

We have to average the last oscillating function over the normal distribution that describes the hyperfine field.

\[
P_r^{2\text{I}}(\tau_s) = \frac{1}{\sqrt{2\pi\sigma_\omega}} \int_{-\infty}^{\infty} d\omega \cos^2 \left( \omega \tau_s \right) e^{-\frac{\omega^2}{2\sigma_\omega^2}} = \frac{1}{2} + \frac{1}{2} e^{-8(\sigma_\omega \tau_s / \hbar)^2}.
\]

2. Mixing of a \( T^L_{LR} \) state with three \( S^L_{LR} \) states - Analytical approach

The effective HFI Hamiltonians \( H_e^{2\text{I}} \) and \( H_e^{2\text{II}} \) presented above (and also the intermediate situations we find for \( \Delta_{so} \) in a perpendicular magnetic field) can be mapped to the problem of dephasing in a non-valley degenerated DQD as the one given in Eq.(37) and Eq.(39c). Here we present the derivation of the latter case and then we particularize for the three mentioned cases.

The electron spin in each dot (\( \xi = L, R \)) follows the evolution operators,

\[
U^\xi(\tau_s) = \cos (\omega_\xi \tau_s) \sigma_0 - i \sigma \cdot \hat{n}_\xi \sin (\omega_\xi \tau_s),
\]

where \( \hat{n}_\xi = \hat{c}_\xi^\dagger \hat{c}_\xi \) is the number operator of the electron spin, \( \omega_\xi = g_\xi (\hat{S}^z - \sigma_z / 2) / \hbar \), \( g_\xi \) is the effective Landé g-factor, and \( \sigma = \sigma_x + i \sigma_y \). We use the symbol of Pauli matrices \( \sigma \). The effective hyperfine Hamiltonian \( H_{eff} = \sum \omega_\xi \sigma \cdot \hat{n}_\xi \) is represented in Eq.(39c).

\[
H_{eff}^{2\text{I}} = \begin{pmatrix} 2\delta h_z^{(0)} & 0 \\ 0 & -2\delta h_z^{(0)} \end{pmatrix}.
\]

In the laboratory frame, the electron is initially prepared in the LR-even state \( \text{LR}_{n,n'}^{even} \). However, due to the dephasing term \( \sigma \cdot \hat{n}_\xi \), in the LR-even state, which has been shown to reduce the spin polarization \( \sigma_z \).

We show that the spin polarization is reduced because the number of electron spin operators \( \sigma_z \) is reduced, which is equivalent to the presence of an effective magnetic field in the presence of the dephasing term. The final result is:

\[
P_r^{2\text{I}}(\tau_s) = \frac{1}{\sqrt{2\pi\sigma_\omega}} \int_{-\infty}^{\infty} d\omega \cos^2 \left( \omega \tau_s \right) e^{-\frac{\omega^2}{2\sigma_\omega^2}} = \frac{1}{2} + \frac{1}{2} e^{-8(\sigma_\omega \tau_s / \hbar)^2}.
\]
that describe precession around the direction of the hyperfine field with frequencies,

\[ \omega_l = \frac{1}{R} \sqrt{(h_{x,\xi})^2 + (h_{y,\xi})^2 + (h_{z,\xi})^2}. \quad (A6) \]

The normalized vectors in Eq.(A5) point in the direction of the local hyperfine field.

\[ \hat{n}_\xi = \frac{1}{h\omega_\xi} (h_{x,\xi}, h_{y,\xi}, h_{z,\xi}). \quad (A7) \]

Using the former evolution operators it follows that an (1,1) Slater determinant in the double dot evolves as,

\[ U(\tau_s) \left| \frac{R,\sigma_R}{\tau_{\sigma_L}} \right. = \sum_{\sigma_1,\sigma_2} U_{\sigma_1,\sigma_2}^{R,L} (\tau_s) U_{\sigma_2,\sigma_R}^{L,R} (\tau_s) \left| \frac{R,\sigma_L}{\tau_{\sigma_L}} \right. \]. \quad (A8) \]

At \( \tau_s = 0 \) the system is initialized in \( T_0^{LR}\text{spin} \), the only available LR-symmetrical state in Eq.(38). In order to time evolve the last two-particle state, we use its Slater determinant version, \( \left\{ |R\rangle + \left| L\right\rangle \right\} / \sqrt{2} \). We apply the evolution operator of Eq.(A8) and project the result back to the initial LR-even state.

\[ \sqrt{p_{\xi}(\tau_s)} = \langle T_0^{LR}\text{spin} | U(\tau_s) | T_0^{LR}\text{spin} \rangle = \frac{1}{2} \left( U_{\uparrow\uparrow}^{LR} U_{\uparrow\downarrow}^{LR} + U_{\uparrow\downarrow}^{LR} U_{\downarrow\uparrow}^{LR} - U_{\downarrow\downarrow}^{LR} U_{\uparrow\uparrow}^{LR} + U_{\downarrow\uparrow}^{LR} U_{\uparrow\downarrow}^{LR} \right) = \cos (\omega_s \tau_s) \cos (\omega_l \tau_s) + \sin (\omega_s \tau_s) \sin (\omega_l \tau_s) h_{\sigma_R} \frac{h_{x,R} h_{x,L} + h_{y,R} h_{y,L} + h_{z,R} h_{z,L}}{h_{\sigma_L}}. \quad (A9) \]

The probability of finding the system in the original state—i.e., of measuring its (0,2) partner state after the adiabatical joining stage—is then the square of the former amplitude.

Since the probability density functions of the hyperfine field components (Gaussian distributions with zero mean) are even, the odd powers terms in those components within \( p_{\xi}(\tau_s) \) do not contribute to the average. We arrive to the well known expression:

\[ P(\tau_s) = \langle \cos^2 (\omega_l \tau_s) \rangle_{L-HF} \langle \cos^2 (\omega_s \tau_s) \rangle_{R-HF} + \sum_{j=x,y,z} \left[ \left( \frac{h_j}{h_{\omega_l}} \right)^2 \sin^2 (\omega_l \tau_s) \right]_{L-HF} \left[ \left( \frac{h_j}{h_{\omega_R}} \right)^2 \sin^2 (\omega_s \tau_s) \right]_{R-HF}, \]

where \( \langle q (h_{x,\xi}, h_{y,\xi}, h_{z,\xi}) \rangle_{\xi-HF} \) stands for the average of the function \( q (h_{x,\xi}, h_{y,\xi}, h_{z,\xi}) \) over the hyperfine fields of the \( \xi \) (L or R) dot. The probability density function (in the 3-dimensional space of \( h_{x,\xi}, h_{y,\xi} \) and \( h_{z,\xi} \)) is

\[ F_{3D} (h_{x,\xi}, h_{y,\xi}, h_{z,\xi}) = \frac{1}{\sqrt{2\pi} \sigma_{h_{x,\xi}}} \sqrt{2\pi} \sigma_{h_{y,\xi}} \sqrt{2\pi} \sigma_{h_{z,\xi}} \exp \left[ -\frac{1}{2} \left( \frac{h_{x,\xi}^2}{\sigma_{h_{x,\xi}}} + \frac{h_{y,\xi}^2}{\sigma_{h_{y,\xi}}} + \frac{h_{z,\xi}^2}{\sigma_{h_{z,\xi}}} \right) \right]. \quad (A11) \]

Where we have used the following standard deviations of the Gaussian distributions for the HFI components,

\[ \sigma_{h_{x,\xi}} \equiv \text{Std}(h_{x,\xi}) , \quad \sigma_{h_{y,\xi}} \equiv \text{Std}(h_{y,\xi}) , \quad \sigma_{h_{z,\xi}} \equiv \text{Std}(h_{z,\xi}). \]

We see below that the degree of anisotropy arising from a difference in the last quantities affects the averages in Eq.(A10) and therefore the return probability.

a. Statistical isotropic 3-dimensional effective hyperfine field

When the effective Hamiltonian is \( H_{\text{eff}}^{3D} \), the three hyperfine components share the same standard deviation, \( \sigma_{h_{x,\xi}} = \sigma_{h_{y,\xi}} = \sigma_{h_{z,\xi}} \), and therefore,

\[ \langle q (h_{x,\xi}, h_{y,\xi}, h_{z,\xi}) \rangle_{\xi-HF} = \int_{-\infty}^{\infty} dh_{x,\xi} \int_{-\infty}^{\infty} dh_{y,\xi} \int_{-\infty}^{\infty} dh_{z,\xi} Q (h_{x,\xi}, h_{y,\xi}, h_{z,\xi}) F_{3D} (h_{x,\xi}, h_{y,\xi}, h_{z,\xi}) \]

\[ = \int_0^\pi d\theta \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi \int_0^{+\infty} dr Q (r, \theta, \varphi) F_{3D} (r, \theta, \varphi), \quad (A13) \]

\[ F_{3D} (r, \theta, \varphi) = \frac{r^2 \sin (\varphi)}{\sqrt{2\pi} \sigma_{h_{x,\xi}}} \exp \left( -\frac{r^2}{2 \left( \frac{h_{x,\xi}^2}{\sigma_{h_{x,\xi}}} \right)} \right), \quad (A14) \]

where we have made a change to spherical coordinates with \( r^2 = (h_{x,\xi})^2 + (h_{y,\xi})^2 + (h_{z,\xi})^2 \).
The two types of averages that appear in Eq. (A10) are obtained by integrating,

\[ C_{3D}(\tau_s) \equiv \langle \cos^2(\omega_s \tau_s) \rangle_{\xi-\text{HF}} = \frac{1}{2} \left( 1 + g \left( \tau_s \sigma^z_{41}/\hbar \right) \right), \quad (A15) \]

\[ S_{3D}(\tau_s) \equiv \left( \frac{h_s \xi}{\hbar \omega} \right)^2 \sin^2(\omega_s \tau_s) \] \[ \xi-\text{HF} \]

\[ = \frac{1}{6} \left( 1 - g \left( \tau_s \sigma^z_{41}/\hbar \right) \right), \quad (A16) \]

\[ g(x) \equiv e^{-2x^2} \left( 1 - 4x^2 \right), \quad (A17) \]

Since \( \hbar \omega_{\xi} = r \) the arguments of the sinusoidal functions in spherical coordinates is \( r \tau_s/\hbar \). Note that in \( S_{3D} \) the average is independent of the direction of the hyperfine component \( (j = x,y,z) \). This is valid here because the effective hyperfine field is statistically isotropic. Then, for simplicity, the integral is computed using the z-component, \( h_{j,\xi} = r \cos(\theta) \).

In the investigated situations in Sec.IV the standard deviations are equal in the two dots, \( \sigma_{41} = \sigma^R_{41} = \sigma^L_{41} \); the return probability becomes

\[ P^4_1(\tau_s) = \frac{1}{3} \left( 1 + g \left( \tau_s \sigma^z_{41}/\hbar \right) + g^2 \left( \tau_s \sigma^z_{41}/\hbar \right) \right). \quad (A18) \]

b. Statistical isotropic 2-dimensional effective hyperfine field

As discussed in Sec.II A 1 the effective Hamiltonian \( H^z_{\text{HF}} \) can be mapped to the GaAs zero-field double dot but it must be assumed that the effective z-component of the hyperfine field is absent. As \( h_{z,\xi} \) is identically zero we must not average over it, therefore, instead of the probability density function given in Eq. (A11) a two dimensional probability density function must be used. Adding the fact that the standard deviations of the in-plane components are identical, \( \sigma^z_{41} = \sigma_{n,\xi} = \sigma_{y,\xi} \), it becomes useful to work in polar coordinates. The averages are obtained as follows,

\[ \langle Q (h_{x,\xi}, h_{y,\xi}) \rangle_{\xi-\text{HF}} = \int dh_{x,\xi} dh_{y,\xi} Q (h_{x,\xi}, h_{y,\xi}) F_{2D} (h_{x,\xi}, h_{y,\xi}) \]

\[ = \int_0^{2\pi} d\varphi \int_0^{+\infty} rQ (r, \varphi) F_{2D} (r, \varphi), \quad (A19) \]

\[ F_{2D} (r, \varphi) = \frac{r}{\left( \sqrt{2\pi} \sigma^z_{41} \right)^2} \exp \left( - \frac{r^2}{2 \left( \sigma^z_{41} \right)^2} \right). \quad (A20) \]

Then we define the 2-dimensional averages needed to compute the return probability as:

\[ C_{2D}(\tau_s) \equiv \langle \cos^2(\omega_s \tau_s) \rangle_{\xi-\text{HF}}, \quad (A21) \]

\[ S_{2D}(\tau_s) \equiv \left( \frac{h_{j,\xi}}{\hbar \omega} \right)^2 \sin^2(\omega_s \tau_s) \] \[ \xi-\text{HF} \]

\[ j = x, y. \]

As in \( S_{3D} \) the average in \( S_{2D} \) is independent of the direction of the hyperfine component \( (j = x, y) \). This is valid here because the effective in-plane hyperfine field is statistically isotropic. Then, for simplicity, the integral is computed using the x-component, \( h_{j,\xi} = r \cos(\varphi) \). The obtained results are presented and discussed in Sec.II A 1.

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