Double quantum dots in carbon nanotubes.

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We study the few-electron eigenspectrum of a carbon-nanotube double quantum dot with spin-orbit coupling. Exact calculation are combined with a simple model to provide an intuitive and accurate description of single-particle and interaction effects. For symmetric dots and weak magnetic fields, the two-electron ground state is antisymmetric in the spin-valley degree of freedom and is not a pure spin-singlet state. When double occupation of one dot is favored by increasing the detuning between the dots, the Coulomb interaction causes strong correlation effects realized by higher orbital-level mixing. Changes in the double-dot configuration affect the relative strength of the electron-electron interactions and can lead to different ground state transitions. In particular, they can favor a ferromagnetic ground state both in spin and valley degrees of freedom. The strong suppression of the energy gap to a ferromagnetic state can cause the disappearance of the Pauli blockade in transport experiments and thereby also limit the stability of spin-qubits in double dots based quantum information proposal. Our analysis is generalized to an array of coupled dots which is expected to exhibit rich many-body behavior.

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I. INTRODUCTION

Experiments on few-electron double quantum dots allow the measurement and manipulation of the spin degree of freedom of the confined electron. Such control is at the heart of semiconductor-based spintronics and quantum-information proposal. Recently, substantial experimental efforts have been focussed on controlling electrons in carbon nanotube double quantum dots, and many of the capabilities previously achieved in GaAs double dots are starting to be reproduced. These include the ability to start from an empty double dot and systematically fill it with electrons. Since C has no nuclear spin, carbon based nanostructures are expected to reduce hyperfine induced decoherence as compared with GaAs.

Furthermore, carbon based materials exhibit richer physics than GaAs semiconducting materials because of the additional valley degree of freedom. In principle, the spin and valley degrees of freedom could lead to a SU(4) symmetry at zero magnetic field instead of the standard SU(2) symmetry in conventional semiconductors (see e.g. Ref. and references therein). However, it has been recently demonstrated that the enhancement of the spin-orbit splitting in small-radius nanotubes breaks the four-fold degeneracy of the single-electron ground state into a two-fold degeneracy.

In this work, we study how spin-orbit coupling and electron-electron interaction effects are manifested in the two-electron spectrum and transport properties of a carbon nanotube double dot. This represents an extension of previous studies on few-electron physics in a single carbon nanotube dot. We find that, despite of spin-orbit coupling and the existence of an additional valley degree of freedom, the two-electron eigenstates can be separated in an orbital part and a spin-valley part that are, to a very good approximation, independent of each other. The spin-valley part can be grouped in ten antisymmetric and six symmetric spin-valley eigenstates which we refer to as multiplets.

The separation of spin-valley degrees of freedom significantly simplifies the description of the systems and allows us to draw analogies with standard GaAs double dots. Our main results can be summarized as follows: (a) For dots at zero magnetic field and no detuning, each dot is populated by a single electron and tunneling is suppressed because of Coulomb interactions. Thus, interdot coupling only occurs virtually via superexchange interactions that determine the ground state symmetry. In this regime, we find a spin-valley antisymmetric ground state, that does not have a well defined-spin due to the spin-orbit coupling. (b) For large detuning between the dots, double occupation of the same dot becomes favorable. In this regime, Coulomb interactions can mix higher orbitals in the two-electron ground state. This admixture significantly reduces the energy spacing between the multiplets (which, for weakly interacting electrons, is determined by the orbital level spacing). The interplay between spin-orbit coupling and interaction then leads to a ferromagnetic ground state above a small critical magnetic field, since the Zeeman terms overcome the strongly suppressed splitting between effective singlet an triplet. c) The reduction of the energy gap between orbitally symmetric and antisymmetric states caused by the Coulomb interaction affects transport properties through the dot and can lead to the disappearance of the so-called Pauli-blockade (suppression of current through the double dot due to the Pauli exclusion principle) and might explain the absence of Pauli blockade reported in Ref. 11. The absence of spin-blockade might affect the performance of quantum information proposal which use spin-qubits in double dots, since gate operation in those proposals is
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based on the spin-blockade mechanism. The disappearance of Pauli blockade might be prevented by reducing Coulomb correlations by either working with short dots, or by covering the nanotube by large dielectrics.

This paper is organized as follows. In the section II, we introduce the microscopic model for the double dot and analyze the non-interacting predictions taking into account a magnetic field parallel to the nanotube axis, spin-orbit couplings and detuning between the dots. Then, we construct a simple two-electron model that captures the interaction effects. This model is then compared with solutions of an exact many-band Hamiltonian using localized single-particle orbitals. In Section III, we discuss the energy spectrum of two interacting electrons in a double dot in three different detuning regimes corresponding to (i) a symmetric double dot, with one electron in each dot, (ii) strong detuning, with both electrons in the same dot, and (iii) at the crossover between both regimes. We then analyze the transport properties of the double dot. Finally, we discuss how to extend our low energy behavior analysis to serially coupled quantum dots. In section IV, we present the conclusion. Technical details on the calculation of Coulomb matrix elements and the derivation of the rate equations used for transport are presented in Appendices A and B.

II. MODEL

Single-wall carbon nanotubes are formed by a single layer of graphite called graphene rolled up into a cylinder. Graphene has a honeycomb lattice formed by covalently bonded carbon atoms. Its electronic properties are determined by the $p_z$ orbital of the carbon atom. The low energy spectrum of graphene consists of two Dirac cones located at the $K$ and $K' = -K$ points of the graphene’s Brillouin zone, where the valence and conduction bands touch. To characterize the two Dirac cones, we introduce the valley index $\tau = \pm 1$, where $\tau = 1$ corresponds to the $K'$ point and $\tau = -1$ to the $K$ point. The behavior of graphene in the presence of an external potential can be described by an effective mass approximation, or $\vec{r} \cdot \vec{p}$ theory\textsuperscript{21}. In this approximation, the envelope wave function for the $A$ and $B$ sites of the two-atom unit cell in a honeycomb lattice follows an effective Dirac equation. In a carbon nanotube, the cylindrical structure imposes a quantization condition that leads to either metallic or semiconducting nanotubes, depending on the orientation of the underlying lattice with respect to the symmetry axis of the tube. Here, we will focus on the behavior of semiconducting nanotubes.

A. Single particle spectrum and interactions

In this section we follow previous work\textsuperscript{12,18,22} to derive the localized eigenstates of a semiconducting nanotube with an additional confinement potential along the tube, which is controlled by external gates. We describe the confinement potential of each dot by a square well (see Fig. 1). The form of the confinement potential will not affect our results qualitatively and we note that for a single dot, the results for parabolic confinement and square well are in good agreement\textsuperscript{18,20}. The external potential leads to a discrete set of bound states. Taking $\zeta$ as the direction of the nanotube axis and $\varphi$ as the angle perpendicular to the nanotube axis, we can write the single particle Hamiltonian as

$$H_0 = -i\hbar v(\tau \sigma_1 \frac{1}{R} \partial_\varphi + \sigma_2 \partial_\zeta) + V(\zeta),$$

where $v$ is the Fermi velocity, $\sigma_i$ are the Pauli matrices operating over the sublattice space, and $V(\zeta)$ is the external potential that describes one or two dots. The eigenstates are determined by matching the solutions for the dot and barrier regions, which are of the form:

$$\Psi^{\tau,\kappa,k}(\varphi, \zeta) = e^{i(kR \varphi + \kappa \zeta)} \left( \frac{z^{\tau,\kappa,k}}{1} \right).$$

Here $\kappa,k$ denote the wave vectors around and along the tube, $z^{\tau,\kappa,k}_\kappa = \pm i(\tau \kappa - ik)/\sqrt{\kappa^2 + k^2}$, and the energy is given by $E_{\kappa,k} = \pm \hbar v \sqrt{\kappa^2 + k^2}$. Solving the effective Dirac equation for $V_{1D}(\zeta)$, which is 0 for $0 < \zeta < L$.
and \( V_g \) otherwise, leads to a quantization condition for the longitudinal momentum modes \( k_n \) of the localized states, where \( n \) denotes the band index.

So far, the \( K \) and \( K' \) solutions are degenerate and independent of spin, \( \sigma = \uparrow, \downarrow \), leading to a four-fold symmetry. However, this symmetry is broken by spin-orbit coupling corrections \( \Gamma_{\text{SO}} \) and by a constant magnetic field \( B \) along the nanotube axis \( \hat{z} \). The spin-orbit coupling and the presence of a magnetic field modify the quantization condition in the \( \hat{z} \) direction,

\[
\kappa = \kappa_0 + \Phi_{\text{AB}}/\Phi_0 R - s\Delta_{\text{SO}}/(\hbar v)
\]

\[
\kappa_0 = \tau/3R.
\]

Here, \( s = \pm 1/2 \) is the quantum number corresponding to the spin operator parallel to the nanotube \((S_z, |\uparrow\rangle = 1/2|\uparrow\rangle \) and \( S_z, |\downarrow\rangle = -1/2|\downarrow\rangle \)); \( \Delta_{\text{SO}} \approx 1\text{mV}/R|\text{nm}| \) is the energy splitting due to spin-orbit coupling, \( \Phi_{\text{AB}} = \Phi_B R^2 \) is the Aharonov-Bohm flux through the nanotube \( R \) and \( \Phi_0 = \hbar e/c \). The magnetic field also leads to a spin Zeeman term \( H_z = sh\omega \), where \( \omega = |e|gB/(2m_0c) \) is the Zeeman frequency in terms of the gyromagnetic constant \( g \), the electron mass \( m_0 \), and the speed of light \( c \). The sign convention for the spin used here is opposite to the one of Ref. 18. Note that in Eq. (4) we only consider the lowest mode in the transverse direction, since excitations involve energies of about \( h\omega/R \) which are much larger than longitudinal-excitation energies or Coulomb-interaction effects as long as \( R \ll L \).

An example of the single particle energy spectrum of a single dot is shown in Fig. 2. Note that we measure the energy with respect to the center of the gap, so that the dominant part of the single-particle energy is constant and given by \( \hbar\omega \approx 220 \text{meV}/R|\text{nm}| \). Generally, disorder or the confinement potential itself can lead to intervalley coupling. However, for a noticeable effect, the potential must change on the scale of the nearest neighbor lattice spacing between carbon atoms \( a_0 = 1.4 \, \text{Å} \). The experiment of Ref. 17 shows only a tiny valley mixing, and we neglect intervalley scattering in this work.

The longitudinal wave vector depends indirectly on spin-valley quantum numbers and on magnetic field and these effects are included in the multi band calculations. However, since \( \kappa_0 \gg \Phi_{\text{AB}}/\Phi_0 R, \Delta_{\text{SO}}/(2\hbar v) \), the single particle energies can be significantly simplified, yielding

\[
E_{n,\alpha} \approx E_n(V_g) + E_{\alpha}
\]

\[
E_{\alpha} = B(\tau_0 \mu_{\text{orb}} + 2\mu_{\text{spin}}s) - \Delta_{\text{SO}} \tau s.
\]

Here we have introduced a single quantum number \( \alpha \equiv (s, \tau) \) to describe the spin valley degrees of freedom \( (\alpha = \uparrow K, \uparrow K', \downarrow K, \downarrow K') \). The confinement energy \( E_n(V_g) = \hbar v\sqrt{s^2 + n^2} \) is the single-particle spectrum of a dot with potential depth \( V_g \) ignoring magnetic field, spin, and spin-orbit dependences; \( \mu_{\text{spin}} = \hbar\omega/(2B) = \hbar|e|g/(4m_0c) \) and \( \mu_{\text{orb}} = (\pi R|e|/\hbar c) \). Within this approximation the orbital part of the single-particle states separate from the spin-valley part. Figure 2 illustrates that, for the parameters studied in this work, spin-valley splitting is basically the same for all longitudinal bands, and Eq. (5) provides a good description of the single-particle spectrum of a single dot.

Next, we consider a biased double-dot system, schematically presented in Fig. 4. In experiment the double quantum dot is formed by applying appropriate voltages to external gates and we model the resulting confinement potential \( V_{2D}(\zeta) \) by a square well potential that is \( -\Delta/2 \) for \( -a/2 \leq \zeta < -a/2 + L \), \( \Delta/2 \) for \( a/2 < \zeta < a/2 + L \), and \( V_g \) otherwise. The length of the dots is \( L \) and \( a \) is the width of the interdot barrier. As discussed previously we do not expect our results to change qualitatively, if a smoother potential is used. In the double-dot system at finite detuning, the depths of the dots change affecting the single particle energies. In the numerical calculation, we determine the eigenspectrum of \( V_{2D} \) exactly. The main effect of the detuning is an energy shift \( \pm \Delta/2 \) to the single-particle eigenenergies, where “+” corresponds to right dot, and “−” to the left dot. Using Eq. (5) and neglecting interdot tunneling, the energies of the localized left and right single-particle orbitals are approximately

\[
E_{n,\alpha}^{L/R} \approx E_n(V_g \pm \Delta/2) + E_{\alpha} \approx E_n(V_g) \pm \Delta/2 + E_{\alpha}.
\]

When more than one electron is confined in the single or double dot, electron-electron interactions become important. The electrons interact through the long-range interactions...
Coulomb potential
\[ V_c(r_1, r_2) = \frac{e^2}{k_d |r_1 - r_2|}, \]  
where \( k_d \) denotes the dielectric constant. Coulomb interactions allow for certain off-diagonal matrix elements in valley space that are produced by intervalley scattering. However, these matrix elements are small for quantum dots with a size much larger than the interatomic distance; they are neglected in this work.

To obtain an accurate description of interacting few electron systems, we extend the single-dot treatment of Refs. \[18,19\] to the double dot system. We construct single particle orbital localized in the left and right dots from the exact single particle solutions of the double dot and we used them to expand the many-body Hamiltonian (see more details in Appendix A). The single particle orbitals have a weak dependence on the spin-valley degrees of freedom that comes from the dependence of the wave vectors \( \kappa \) and \( k \) on \( \tau \) and \( s \). This leads to a dependence of the interaction matrix elements on the spin-valley degrees of freedom. However, this dependence is very weak and, to a very good approximation, can be neglected. Thus, interactions can be considered spin-valley independent which allows a separation of orbital and spin-valley contributions of the two-electron solutions.\[18\]

### B. Separating orbital from spin-valley degrees of freedom

Since interactions can be considered diagonal in spin-valley degrees of freedom, orbital and spin-valley part of the two-electron solutions provide independent contributions to the energies and the wave functions. The total two-particle wave function must be antisymmetric with respect to particle exchange and the symmetry of the orbital part must always be opposite to that of the spin-valley part. Thus, the two-particle spectrum can be grouped according to their orbital symmetry or parity under particle exchange in multiplets of six states if the orbital part is symmetric or ten states if the orbital part is antisymmetric. The energy splitting between different multiplets, called \( \epsilon \), depends on the orbital part, which is determined by electron-electron interactions and longitudinal confinement, and it is generally given by a correlated state that is represented as a superposition of various two-electron orbital wave functions. The energy relations within a multiplet are exclusively determined by \( E_\alpha \), which includes the orbital and spin Zeeman terms as well as the spin-orbit coupling Eq. \[1\]. Therefore, the spin-valley part of the wave function always has the simple form shown in Table \[3\].

The magnetic field dependence of the two multiplets is illustrated in Fig. \[3\]. The competition between spin-orbit coupling and orbital Zeeman energy leads to a ground state crossings in the orbital part with antisymmetric spin-valley part at a critical magnetic field \( B_c = \Delta_{SO}/2\mu_{orb} \). For \( B < B_c \) the ground state of the antisymmetric spin-valley multiplet (Fig. \[3\] (a)) is in a superposition of singlet and triplet, since \( |K\downarrow, K'\uparrow\rangle = (|KK'\uparrow\rangle - |KK'\downarrow\rangle)/\sqrt{2} \). For \( B > B_c \), the lowest state of the antisymmetric spin-valley multiplet \( |KK'\uparrow\rangle \) is a superposition of spin and valley space for all positive magnetic fields.

The energy difference between the different multiplets \( \epsilon \) and the magnetic field \( B \) determines the spin-valley symmetry of the ground state. The thick curves in Figs. \[3\] (a) and (b) correspond to the possible ground states which we label according to their spin and valley symmetry.

### C. Model Description

One of the objectives of this study is to be able to describe the evolution of the spectrum as the detuning is changed from small to large and the low energy configurations change from \([1L, 1R]\), i.e. one electron per dot, to \([2L, 0R]\) or \([0L, 2R]\), two electrons in the same dot. An accurate description of the strong interaction effects requires the inclusion of several single particle bands of the double dot system. For example, the behavior of the \([2L, 0R]\) configurations is expected to be very similar to that of the doubly occupied single dot and in that situation the strong correlations need to be described by many single particle orbitals.\[18,19\] This situation makes the description and the interpretation of the results not very intuitive. However, we can significantly simplify the description by realizing that no matter how strongly correlated the system is, the parity is a good quantum number and the states can be classified according to the state parity. Thus, we can model the exact system with a sim-
ple effective Hamiltonian in the charge degrees of freedom that captures this dependence on parity and describes the energetically lowest multiplets of the $|1L,1R\rangle$, $|2L,0R\rangle$ and $|0L,2R\rangle$ configurations.

The charge degrees of freedom of two-electrons in a double dot can have three configurations: $|2L,0R\rangle^\pm$, $|1L,1R\rangle^\pm$, and $|0L,2R\rangle^\pm$, where $\pm$ characterizes the conserved orbital symmetry (i.e. + for antisymmetric spin-valley states and - for symmetric spin-valley states). Within this model, interaction effects can be obtained by diagonalizing the effective Hamiltonians $H_S$ and $H_{AS}$, where $S$ and $AS$ denote symmetric and antisymmetric spin-valley state. The complex multiband problem is then reduced to simple 3 times three matrices.

$$H_S = \begin{pmatrix} V + V_{ex} - \Delta & -t_S & 0 \\ -t_S & V_{LR} & t_S \\ 0 & t_S & V + V_{ex} + \Delta \end{pmatrix}$$  \hspace{1cm} (9)$$

and

$$H_{AS} = \begin{pmatrix} V - V_{ex} - \Delta & -t_{AS} & 0 \\ -t_{AS} & V_{LR} & -t_{AS} \\ 0 & -t_{AS} & V - V_{ex} + \Delta \end{pmatrix}.$$  \hspace{1cm} (10)

These effective Hamiltonians include the onsite and nearest neighbor interactions $V$ and $V_{LR}$, the tunnelings in symmetric $t_S$ and antisymmetric $t_{AS}$ configuration and the detuning effects $\Delta$. The dependence of the interaction on the symmetry is introduced by an effective exchange term $V_{ex}$ that favors the antisymmetric spin-valley configuration. Equations 9 and 10 describe the energy related with the orbital part of the wavefunction. The total energy also contains the contribution of the spin-valley part $E_{SV} = \sum_{\alpha}|E_{\alpha}(V_{\alpha}) + E_{\alpha}|n_{\alpha}$, where $E_{\alpha}$ was defined in Eq. (6) and $n_{\alpha}$ denotes the occupation of states with spin-valley $\alpha$.

To gain qualitative understanding of the interaction and tunneling terms in the effective Hamiltonian, we analyze the limiting behaviors of the low-energy spectrum. First, we consider the limit of zero detuning and large local Coulomb interactions and we obtain that the lowest symmetric and antisymmetric spin-valley multiplets have energies:

$$E_{AS}^g \approx E_{SV} + V_{LR} - \frac{2t_{AS}^2}{V - V_{LR} - V_{ex}} + \ldots,$$  \hspace{1cm} (11)

$$E_S^g \approx E_{SV} + V_{LR} - \frac{2t_S^2}{V - V_{LR} + V_{ex}} + \ldots.$$  \hspace{1cm} (12)

In this limit, energies of the lowest symmetric and antisymmetric spin-valley multiplets are

$$E_{AS}^g \approx E_{SV} - \Delta + V - V_{ex} + \ldots,$$  \hspace{1cm} (13)

$$E_S^g \approx E_{SV} - \Delta + V + V_{ex} + \ldots,$$  \hspace{1cm} (14)

Thus, the energy splitting $\epsilon = E_S^g - E_{AS}^g \approx 2V_{ex}$ in the $(2,0)$ configuration is mainly controlled by the exchange mechanism.

This effective model allows a simple and intuitive understanding of the underlying physical behavior of the double dot system. However, to extract the parameters $V, V_{LR}, V_{ex}$ and $t_{12}$ we need to solve exactly the single and double dot system. In the next Section, we analyze the behavior of the double-dot system at different magnetic field, detuning and interaction regimes by comparing the exact diagonalization solutions discussed in the previous subsection with the model Hamiltonian. From this comparison, we extract the parameters of the model.

### III. RESULTS

In this section, we analyze the energy spectrum of two interacting electrons in a double dot in three different detuning regimes: (A) small detuning, with one electron in each dot; (B) strong detuning, with both electrons in the same dot and (C) at the crossover between both regimes. In subsection 11D we study the transport properties of the double dot.

The analysis of the spectrum and transport properties is characterized the energy spacing $\epsilon$ which can be defined in the exact calculations as the energy difference between the lowest energy state with an antisymmetric orbital part and and the lowest state with a symmetric orbital part at zero magnetic field $B = 0$. In all detuning regimes, we find $\epsilon > 0$, in agreement with the Lieb Mattis theorem. However, Coulomb correlations can significantly reduce $\epsilon$.

In our analysis, we have considered different double dot configurations by changing the length and depth of the dots as well as the interdot distance and found the same scaling of interaction effects as discussed in Ref[18]. In this section we present results for the parameters $L = 70$ nm, $a = 20$ nm, $V_g = 78$ meV, $R = 2.5$ nm. These parameter lead to an energy splitting between the two lowest single-particle longitudinal modes of $\hbar \omega_0 \approx 10.6$ meV and the symmetric double dot supports five bound states per quantum dot that are all included in the multi-band calculation. The dielectric constant $\kappa_d$ is varied between $1.5 < \kappa_d < 3.5$ which allows us to explore the strongly interacting regime where new transitions occurs. Experimentally, however, it is easier to change the length of the dots. The parameter that characterize the strength of the interactions is the ratio $U/(\hbar \omega_0)$ between typical single particle excitation energies $\hbar \omega_0$ and the typical intradot interaction energy scale $U = e^2/k_d L$. This ratio is typically $1 < U/(\hbar \omega_0) < 5$.
which imply a moderate/strong interaction regime. Another relevant parameter that determines the regime of a quantum dot is, as we will discuss below, the ratio $2V_{ex}/\Delta_{SO}$ that reflects the competition of strong correlations and spin-orbit effects and determines the spin-valley nature of the ground state.

A. Low energy spectrum of symmetric double dot

![Graph of low-energy spectrum of a double dot as a function of $B$.](image)

**FIG. 4:** (Color online) Low-energy spectrum of a double dot as a function of $B$. Solid symbols (red online) correspond to states belonging to the antisymmetric spin-valley multiplet and open symbols (blue online) to the symmetric spin-valley states belonging to the antisymmetric spin-valley multiplet. The solid curves correspond to the effective Hamiltonian description.

First, we analyze the numerical results obtained with the multiband treatment. Figure 4 shows the low-energy spectrum as a function of $B$ for $k_d = 2.5$ in a double dot with $\Delta = 0$ (zero detuning). In the low-energy spectrum, we can recognize the symmetric and antisymmetric spin-valley multiplets discussed in Table 3. The energy difference $\epsilon$ between the two multiplets is not observable in the energy range of Fig. 4. Since interdot tunneling is very small compared with the interaction energy, the two electrons occupy different dots to avoid strong intradot interactions. The interdot interaction is almost independent of the orbitals occupied in each dot. Thus, at small detuning there is a negligible occupation of higher bands.

In Fig. 4 we identify three states that will be relevant for the discussion of Pauli blockade. One of them has mixed valley-spin symmetry and we label it as $|\tilde{M}\rangle$. The second state is antiferromagnetic in spin and ferromagnetic in valley degree of freedom and we label it as $|\tilde{A}F\rangle$. The third state, labeled $|FF\rangle$, is ferromagnetic in both spin and valley degrees of freedom. States $|\tilde{M}\rangle$, $|\tilde{A}F\rangle$ belong to the antisymmetric spin-valley multiplet and $|FF\rangle$ belongs the symmetric spin-valley multiplet.

Their configurations are approximately

$$|	ilde{M}\rangle \approx |1L,1R\rangle^{\pm} |K\downarrow;K'\uparrow\rangle,$$  
$$|\tilde{A}F\rangle \approx |1L,1R\rangle^{\pm} |K\downarrow;K\uparrow\rangle,$$  
$$|FF\rangle \approx |1L,1R\rangle^{-} |K\downarrow;K\downarrow\rangle. $$  

In the exact diagonalization calculation, we extract the orbital structure and conclude that $|1L,1R\rangle^{\pm}$ is given to a very good approximation by single Slater determinant formed with left and right orbitals in the lowest band.

We can approximate the energies of $|\tilde{M}\rangle$, $|\tilde{A}F\rangle$ and $|FF\rangle$ using Eqs. (7), (11) and (12),

$$E_{\tilde{M}} \approx 2E_{1L}(V_g) - 2t_{12}^2/(V - V_{ex}) + V_{LR} - \Delta_{SO},$$  
$$E_{\tilde{A}F} \approx 2E_{1L}(V_g) - 2t_{12}^2/(V - V_{ex}) + V_{LR} - 2B\mu|\tilde{M}\rangle,$$  
$$E_{FF} \approx 2E_{1L}(V_g) - 2t_{12}^2(V + V_{ex}) + V_{LR} - \Delta_{SO} - 2B(\mu_{orb} + \mu_{spin}).$$

At $B = 0$, the ground state $|\tilde{M}\rangle$ is only separated by the very small superexchange energy $\epsilon \approx 4t_{12}^2V_{ex}/V^2$ from the lowest spin-valley symmetric triplet that contains $|FF\rangle$. These four states are separated from the rest of the spectrum by a much larger energy scale given by $\Delta_{SO}$. This energy structure resembles the singlet-triplet splitting in GaAs double quantum dots. At finite fields, $|FF\rangle$ is the ground state. The first excited state changes with increasing magnetic field from $|\tilde{M}\rangle$ to $|\tilde{A}F\rangle$ at $B_c = \Delta_{SO}/(2\mu_{orb})$, as shown in Fig. 4. This crossing between two antisymmetric spin-valley states has no analogous in standard GaAs quantum dots.

From the analysis of the single and double dot spectrum, we can obtain the parameters of the charge effective Hamiltonian (Eqs. 8-10). Figure 5 presents the parameters $V$, $V_{LR}$, $t_{12}$ and $V_{ex}$ for a double dot with $L = 70$ nm, $a = 20$ nm, $V_g = 78$ meV, $R = 2.5$ nm, and $\Delta = 0$. The $V$ and $V_{ex}$ are obtained from the two-electron spectrum in a single dot and $V_{LR}$ and $t_{12}$ obtained from double dot spectrum. The black solid curves in Fig. 4 show the prediction from the model using the
B. Low energy spectrum for large detuning: Two electrons in a single dot

When the detuning is large enough to overcome the intradot interaction, both electrons occupy the same dot, and the charge degree of freedom of the low-energy eigenstates can be described by the \( |2L, 0R\rangle\) configuration. Thus, the energy spectrum resembles the one obtained for two electrons in an isolated dot.\(^\text{[53]}\)

![Graph showing low energy spectrum at large detuning](image)

**FIG. 6:** (Color online) Low energy spectrum at large detuning (\(\Delta \approx 35\) meV). Solid symbols (red online) correspond to states belonging to the antisymmetric spin-valley multiplet, and open symbols (blue online) to the symmetric spin-valley multiplet. Curves represent the model predictions.

Figure 6 presents the low energy spectra for large detuning for \(k_d = 2.5\). The solid curves represent the effective Hamiltonian predictions. The multiband structure of the solutions introduce corrections to the spin-valley dependence of the spectrum which can be absorbed in effective \(\mu_{\text{orb}}\) and \(\Delta_{\text{SO}}\). However, these corrections are small and correspond to a few percent changes to the bare \(\mu_{\text{orb}}\) and \(\Delta_{\text{SO}}\) values.

At zero magnetic field, the antisymmetric spin-valley multiplet is favored. This is in agreement with Lieb Mattis theorem,\(^\text{[53]}\) that states that the two particle ground state always has a symmetric orbital part. In our two-electron system, we can understand this prediction from the analysis of the orbital symmetry of the wave function. In the noninteracting limit, the orbital ground state is constructed with both electrons in the lowest band corresponding to a symmetric orbital wave function, i.e., an antisymmetric spin-valley wave function. To form an antisymmetric orbital wave function at least one electron has to occupy an excited state. Thus, in the noninteracting limit, \(\epsilon\) is given by the level splitting \(\hbar \omega_0\) between the first two bands. However, the energy difference \(\epsilon\) between the two multiplets shown in Fig. 6 is much smaller than \(\hbar \omega_0\). Furthermore, the reduction of \(\epsilon\) with respect to the level splitting is much stronger for smaller dielectric constant or longer dots, since interaction effects are more relevant. In the limit of infinite interactions, the electrons are strongly localized at the positions that minimize the interaction energy. Then the orbital symmetry of the wave function becomes irrelevant and \(\epsilon\) vanishes. This effect is a signature of a formation of a Wigner molecule.\(^\text{[18–20]}\)

In the effective Hamiltonian, the formation of a Wigner molecule is manifested in the reduction of the parameter \(V_{\text{ex}}\). This is evident in Fig. 5 that shows that \(V_{\text{ex}}\) is a growing function of the dielectric constant. Even though the results of Fig. 5 are for \(\Delta = 0\), we note that \(V\) and \(V_{\text{ex}}\) depend weakly on the detuning and can be approximated by \(\Delta = 0\) predictions for all detunings studied here \(\Delta < 35\) meV. In contrast, the tunneling \(t_{12}\) is strongly affected by the detuning and is reduced almost by approximately a factor of two in comparison with the \(\Delta = 0\) case.

The reduction of \(\epsilon\) implies that the exact eigenstates become strongly correlated and cannot be written as non-interacting wave functions to characterize them. However, we can still label the low-lying \((2,0)\) states according to their conserved quantum numbers:

\[
|M\rangle = |2L, 0R\rangle^+ |K \downarrow; K' \uparrow\rangle^-, \quad (21)
\]

\[
|AF\rangle = |2L, 0R\rangle^+ |K \downarrow; K \uparrow\rangle^+, \quad \text{and} \quad (22)
\]

\[
|FF\rangle = |2L, 0R\rangle^- |K \downarrow; K \downarrow\rangle \quad (23)
\]

Here the states \(|2L, 0R\rangle^\pm\) are correlated orbital states of two electrons in the left dot. Our numerical calculations shows that several bands are needed to represent these states accurately. We note that Secchi and Rontani found qualitatively the same correlation effects for a parabolic well with weak confinement,\(^\text{[49]}\) which suggests the robustness of these correlation effects. We note that because of the conserved symmetries, the eigenstates at small detuning \(|M\rangle, |AF\rangle, \text{and} |FF\rangle\) will evolve in \(|M\rangle, |AF\rangle, \text{and} |FF\rangle\) for large detuning.

Using the effective Hamiltonian along with the approximate description of the single particle energies \(\text{Eqs. 7, 13 and 14}\), we can obtain simple expression for the \((2,0)\) configuration energies:

\[
E_{|M\rangle} \approx 2E_L(V_g) + V - V_{\text{ex}} - \Delta_{\text{SO}} - \Delta, \quad (24)
\]

\[
E_{|AF\rangle} \approx 2E_L(V_g) + V - V_{\text{ex}} - 2B\mu_{\text{orb}} - \Delta, \quad \text{and} \quad (25)
\]

\[
E_{|FF\rangle} \approx 2E_L(V_g) + V + V_{\text{ex}} - \Delta_{\text{SO}} - 2B(\mu_{\text{orb}} + \mu_{\text{spin}}) - \Delta. \quad (26)
\]

At \(B = 0\), \(|M\rangle\) is the ground state. Above a critical magnetic field, there is a ground-state transition to either \(|AF\rangle\) \(\Delta_{\text{SO}} < \epsilon\) or \(|FF\rangle\) \(\Delta_{\text{SO}} > \epsilon\) due to the orbital Zeeman term. Thus, the reduction of \(\epsilon\) leads to a ground state transition to the ferromagnetic state \(|FF\rangle\) at finite magnetic field. In practice, the formation of a ferromagnetic ground state can be experimentally controlled by changing the length of the dots.
C. Transition from a double- to a single-dot regime.

We now analyze the transition between the limiting behaviors discussed in the previous two sections.

Figure 7 shows the crossover between $|1L, 1R\rangle$ states and $|2L, 0R\rangle$ states of the double dot system at $B = 0$. In absence of interdot tunneling, the two-electron spectrum shows sharp crossings between the $|1L, 1R\rangle$ states and $|2L, 0R\rangle$ states with increasing detuning. Because of the interdot tunneling, crossings between states with the same symmetries turn into avoided crossings. The avoided crossings occur at the same critical detuning for states of the same multiplet. The avoided crossings within the multiplet with an antisymmetric orbital part occur at relatively larger detuning since the tunneling electron is forced to occupy an excited band.

The crossover regime, presented in Fig. 7, is strongly affected by interactions. The difference between the critical detunings belonging to the avoided crossings of states with symmetric and antisymmetric orbital part is a direct measure for the energy splitting $\epsilon$. Furthermore, correlations in the $|2L, 0R\rangle$ states decrease the tunneling coupling to the corresponding $|1L, 1R\rangle$ state, leading to a sharper avoided crossing.

In the effective Hamiltonian description, the lowest $|1L, 1R\rangle$ and $|2L, 0R\rangle$ configurations are close in energy when $\Delta \sim V - V_{LR}$. In this regime, the $|0L, 2R\rangle$ configurations are energetically suppressed and do not affect the low energy spectrum. Within this approximation, we can obtain a simple expression for $\epsilon$

$$\epsilon = V_{ex} + \frac{1}{2} \left( \sqrt{4t_{12}^2 + (\Delta - V_{ex} - V + V_{LR})^2} - \sqrt{4t_{12}^2 + (\Delta + V_{ex} - V + V_{LR})^2} \right)$$

This expression compares well with the numerical prediction as shown in Fig. 8.

From the analysis of the low-energy spectrum, e.g., Fig. 7, we can extract the phase diagram as a function of the detuning $\Delta$ and the magnetic field $B$. The phase diagrams for strong ($k_d = 1.5$) and weak ($k_d = 3.5$) interactions, presented in Fig. 8, exhibit clear differences. At exactly zero magnetic field, the ground state always has a symmetric orbital wave function ($|M\rangle$ and $|\bar{M}\rangle$). This state is preferred with respect to other states within the same multiplet by the spin-orbit coupling $\Delta_{SO}$ and, with respect to states of the other multiplet, by the energy gap $\epsilon$. The ground state changes at a critical magnetic field to a valley-polarized state. The valley polarized ground state has symmetric orbital part for $\Delta_{SO} < \epsilon$ and an antisymmetric orbital part for $\Delta_{SO} > \epsilon$. For small detuning $\Delta$, the energy splitting $\epsilon$ is caused by the small superexchange and $\epsilon < \Delta_{SO}$. However, for large detuning, both electrons are on the same dot, and the value of $\epsilon$ can be larger or smaller than $\Delta_{SO}$. Thus, if $2V_{ex} > \Delta_{SO}$, there is a transition to a valley-polarized state with a symmetric orbital part, $|AF\rangle$, as detuning is increased [as observed in Fig. 9 (b)].
D. Sequential transport

In this section, we discuss how the two-electron eigen-spectrum affects sequential transport through a double dot. In particular, we analyze the existence of Pauli blockade in a sequential tunneling dot that would lead to a current rectification in DC transport [23]. Figure 10 shows a schematic description of two situations when a Pauli blockade occurs. In both cases, the double-dot system is detuned such that there is always at least one electron in the left dot. States relevant for transport through the double dot are the $|2L, 0R⟩$ states $|M⟩$ and $|FF⟩$ as well as the $|1L, 1R⟩$ states $|M⟩$ and $|FF⟩$. In Fig. 10 the vertical axes denote energy and the horizontal axes denote the spatial coordinate along the nanotube. The center of each figure shows the double dot created by tunnel barriers to the contacts and between the dots. The gray rectangles to the left and right of the double dot are the Fermi seas in the contacts.

(a) $B=0$ Blocked

(b) $B=B^*$ Blocked

FIG. 10: (Color online) Schematic representation of a Pauli blockade for zero magnetic field and negative bias (a), and finite magnetic field and positive bias (b). The white areas in the center of each figure represent the two dots. The black circle in the left dot represent the position and energy of one of the electrons. The states $|M⟩$ and $|M⟩$ are represented by solid lines with $|FF⟩$ and $|FF⟩$ by dashed lines. These states are organized vertically according to their energies and also represent the possible positions of the second electron. The wide gray rectangles next to the left and right dots represent the energy bias.

For a positive bias voltage (opposite to Fig. 10(a)), the electrochemical potential in the left contact is larger than in the right one, and current flows via a sequential tunneling process $|1L, 0R⟩ → |2L, 0R⟩ → |1L, 1R⟩ → |1L, 0R⟩$. Interdot tunneling is assumed to conserve the spin-valley degree of freedom and allows for transitions between states $|M⟩$ and $|M⟩$ or $|FF⟩$ and $|FF⟩$. Because of the sequential transport setup, the left dot couples to the left reservoir, allowing for transitions between the $|1L, 0R⟩$ and $|2L, 0R⟩$ states. Analogously, the right contact allows for transitions between the $|1L, 0R⟩$ and $|1L, 1R⟩$ states. Figure 10(a) considers Pauli blockade at $B = 0$.

In this scenario, the current is blocked when state $|FF⟩$ is occupied by an electron tunneling in from the right reservoir. In fact a $B = 0$ the ground state of the symmetric multiplet is three fold degenerate, but as long as spin and valley are conserved this degeneracy does not change the physics, see Appendix B. Once in state $|FF⟩$, the electron cannot tunnel back because of the filled Fermi sea in the right contact. It also cannot tunnel to the left dot since the corresponding state $|FF⟩$ has much larger energy than state $|FF⟩$ because of the energy difference $\epsilon$ between states $|M⟩$ and $|FF⟩$. However, $\epsilon$ can be strongly reduced, allowing for a finite exit rate from state $|FF⟩$ as shown in Fig. 10(a). This effect might explain the absence of a Pauli blockade in Ref. [11]. This Pauli blockade implies a rectification of the current since, by inverting the bias voltage, a finite current can flow.

In order to make these statements more quantitatively we calculate the stationary current with a rate equation approach [23,29]. We describe the regime of possible blockade depicted in Fig. 10(a) while assuming spin-orbit coupling to be much bigger than temperature, transport voltage and external coupling the two reservoirs.

The rate equations and the resulting stationary current are given in Appendix B. The dependence of the stationary current $I_{on}$ in the blockade setup and the probability to be in any of the three degenerate $|FF⟩$ states are given by:

$$I_{on} = \frac{t_S^2 A}{B + C(2t_S^2 + \epsilon^2)}$$  \hspace{1cm} (28)

$$P_{FF} = \frac{C(t_S^2 + \epsilon^2) + D}{B + C(t_S^2 + \epsilon^2)}$$  \hspace{1cm} (29)

Here $\epsilon$ denotes the energy splitting between the states $|M⟩$ and $|FF⟩$ and $t_S$ is the interdot tunneling rate between states $|FF⟩$ and $|FF⟩$. The constants $A, B, C, D$ depend on the coupling strength to the contacts and spectral weights for the tunneling probabilities and their form is given in Appendix B.

If $\epsilon$, is the dominant energy scale then the current is suppressed as $I_{on} \propto 1/\epsilon^2$ and the double dot gets stuck in states $|FF⟩$ with $P_{FF} \rightarrow 1$. This is the regime of Pauli-blockade. However, we find that due to interaction effects interdot tunneling $t_S$ can even exceed the energy splitting $\epsilon$, thus removing the blockade mechanism.

Due to Pauli-blockade the double dot acts as a current rectifier, since by reversing the transport voltage in Fig. 10 a possible current can flow. Fig. 11 illustrates how effective the double dot acts as current rectifier as function of $\epsilon$.

At finite magnetic field, the transport behavior can also be very interesting. For example, if interactions are strong enough to suppress $\epsilon$ to become on the order of the spin-orbit coupling ($\Delta_{SO} \geq \epsilon$) but still much larger than the interdot tunneling ($\epsilon \gg t$), then a current blockade can occur in the opposite bias direction of the zero field case. This situation is depicted in Fig. 10(b). A magnetic field $B^* \approx \epsilon/2(\mu_{orb} + \mu_{spin})$ is applied so that states $|FF⟩$ and $|M⟩$ are degenerate, while in the $|1L, 1R⟩$ charge configuration, the state $|FF⟩$ is ground state and
that describes two electrons in the $r$ dot can be expanded in single particle basis as

$$|d_{\eta,r,\alpha,\alpha'}\rangle = f_{\alpha,\alpha'}^{-1} \sum_{n \leq m} \beta_{\eta,m,n} (a^\dagger_{r,n,\alpha} a^\dagger_{r,m,\alpha'} + (-1)^n a^\dagger_{r,n,\alpha'} a^\dagger_{r,m,\alpha}) |0\rangle$$  \hspace{1cm} (30)

Here, $\eta$ labels the spin-valley symmetry of the two-electron state $\eta = 1$ for antisymmetric spin-valley states and $\eta = 2$ for symmetric spin-valley states and $f_{\alpha,\alpha'} = \sqrt{1+\delta_{\alpha,\alpha'}}$. Equation (30) defines the doubleon operator such that $|d_{\eta,r,\alpha,\alpha'}\rangle = d^\dagger_{\eta,r,\alpha,\alpha'}|0\rangle$ and $d^\dagger_{\eta,r,\alpha,\alpha'} = (-1)^n d^\dagger_{\eta,r,\alpha',\alpha}$. Note that the $\beta_{\eta,m,n}$ do not depend on $\alpha$ and $\alpha'$. The coefficients $\beta_{\eta,m,n}$ can be obtained by diagonalizing the local part of the Hamiltonian which amounts to solve two electrons in a single dot. We now assume that the occupation of higher excited two-particle states, which are separated by an energy gap of the order of the single particle level spacing, can be neglected. This should be a good approximation for the low energy spectrum.

The effective Hamiltonian is obtained by projecting the complete Hamiltonian onto the subspace of empty, singly and doubly occupied dots and can be written as

$$H_{\text{eff}} = P (H_e + H_d + H_{ed} + V_c) P$$  \hspace{1cm} (31)

where $P \equiv \prod_i P_i$ represent a projector to the physically allowed subspace where $P_i = |0\rangle \langle 0| + \sum_\alpha \langle \alpha |i \rangle \langle i | \alpha + \sum_\eta |d_\eta\rangle \langle d_\eta|$ (see Ref. [22]). $H_e$ describes the behavior of single occupied dots, $H_d$ describes the behavior of double occupied, $H_{ed}$ contains a coupling between singly and doubly occupied dots and $V_c$ represents the Coulomb interaction between different sites. The explicit form of these contributions is:

$$H_e = \sum_{r,\alpha} E_{r,\alpha} a^\dagger_{r,\alpha} a_{r,\alpha} + \sum_{r',\alpha} t_{r,r'} a^\dagger_{r',\alpha} a_{r,\alpha}$$  \hspace{1cm} (32)

$$H_d = \sum_{r,\eta,\alpha \leq \alpha'} E_{2\eta,r,\alpha,\alpha'} d^\dagger_{\eta,\alpha,\alpha'} d_{\eta,\alpha,\alpha'} + \sum_{r',\eta,\alpha \leq \alpha'} t^{(d)}_{\eta,r,r'} d^\dagger_{\eta,\alpha,\alpha'} d_{\eta,r',\alpha,\alpha'}$$  \hspace{1cm} (33)

$$H_{ed} = \sum_{r',r,\alpha,\alpha'} t_{r,r'}' f_{\alpha,\alpha'} a_{r,\alpha} d^\dagger_{\eta,\alpha,\alpha'} d_{\eta,r',\alpha,\alpha'} + \sum_{r',r,\eta,\alpha,\alpha'} f_{\alpha,\alpha'} g_{r,\alpha'} [d^\dagger_{\eta,\alpha,\alpha'} a_{r,\alpha} + H.c]$$  \hspace{1cm} (34)

The diagonal part of $H_e$ and $H_d$ represent the electron and doubleons energies composed of the spin-valley energy and onsite energies ($E_{r,\alpha} = E_\alpha(V_r) + E_\alpha$ and $E_{2\eta,r,\alpha,\alpha'} = 2E_\eta(V_r) + E_\alpha + E_{\alpha'} + V + (-1)^n V_{ex}$) and $t$ and $t^{(d)}$ the tunnelings of the electrons and doubleons. The

E. 1D-Quantum dot arrays

The rich physics associated with the strong correlations of double occupied dots is expected to have significant impact in the many-body behavior of a one-dimensional chain of dots. The double dot analysis carried out here can be used as a starting point to study the behavior of a linear array of coupled dots. According to our analysis, there exists an interaction regime in which the behavior of two electrons in the same dot is strongly correlated and controlled by $\epsilon$ while the interaction between electrons in different dots does not introduce band mixing. In order to generate an effective Hamiltonian that captures the essential effects of strong onsite correlations, we apply the ideas of Hubbard operators to describe double occupied dots or doubleons (see i.e. Ref. [21]). This description assumes that the strong onsite Coulomb repulsion suppresses the probability to occupy a dot with more than two electrons. This is a good approximation for low enough fillings.

Formally, we start from the complete Hamiltonian that describes a chain of dots. This Hamiltonian represents an extension of the double dot Hamiltonian introduced in the Appendix.

We introduce the operators $a^\dagger_{r,n,\alpha}$ which create an electron in the $r$ dot, in the $n$ orbital state and with a given spin-valley configuration $\alpha$. To simplify the notation we introduce $a^\dagger_{r,1,\alpha} \equiv a^\dagger_{r,\alpha}$ for electrons in the lowest band which describe well the singly occupied dots. The state

$FIG. 11$: (Color online) Ratio between leakage current ($I_{\text{on}}$) corresponding to setup in Fig. 10(a) and the finite current for reversed transport voltage ($I_{\text{off}}$). Used parameters $I_{\text{on}} = 0.01\text{meV}$, $t_{\text{AS}} = t_{\text{S}} = 0.1\text{meV}$ and $S_M = 0.7$, $S_F = 1$. 

separated from state $|\tilde{\Psi}\rangle$ by the energy $\epsilon$ (because of the applied field $B$). The physical situation of Figure 10 (b) resembles that of Fig. 10 (a), and also results in a current blockade. The ability to control the direction of the current rectification by varying the magnetic field can have applications to carbon nanotube-based spintronic proposals.
$H_{ed}$ contains a term that describes the hopping of an electron from the doubly occupied site to a singly occupied site which in this language corresponds to an exchange of a doublon and an electron. The second term in $H_{ed}$ represents the hopping of an electron from a singly occupied site to a singly occupied site and vice versa, which is represented as destroying two atoms and creating a doublon. Finally, we have the offsite Coulomb interaction $V_c$ in terms of the dot density $n_r$ defined as

$$n_r = \sum_\{\alpha\} a_{\alpha r}^{\dagger} a_{\alpha r} + 2 \sum_{\eta} \{\alpha, \alpha'\} d_{\eta,\alpha r}^{\dagger} d_{\eta,\alpha r}.$$  \hspace{1cm} (35)

Here, the summation $\{\alpha, \alpha'\}$ is restricted to $\alpha < \alpha'$ for $\eta = 1$ and $\alpha \leq \alpha'$ for $\eta = 2$. For the offsite interaction we assume exclusively capacitive coupling and neglect a dependence on the symmetry of the two particle states.

In the most general case the parameters that describe the effective Hamiltonian depend on lattice sites positions and can be controlled by changing the detuning in each lattice site $\Delta_r$. For example, an enhancement of the superexchange interactions can be achieved by detuning some of the dots and, therefore, reducing the energy cost of double occupancies.

The effective Hamiltonian can be applied to describe an array of coupled dots in many different regimes and its phase diagram might exhibit novel phases. In particular, the existence of spin-valley “triplet” close in energy to the spin-valley “singlet” can lead to phenomena richer in comparison to the standard single-band Hubbard model. For example, for one particle per site (filling $n = 1$), it is known that the ground state of the usual Hubbard model has infinite susceptibility to spin dimerization i.e. formation of singlet/triplet bonds between nearest-neighbor sites. However, the ground state is not dimerized since the formation of singlet bonds, say at sites $(2i, 2i+1)$, is penalized by the large energy cost of the remainder triplet components between sites $(2i+1, 2i+2)$. In carbon nanotubes operating in the strongly interacting regime, $\varepsilon \ll 1$, even spin-valley “triplet” states can lower their energy by virtual hopping. The later situation reduces the energy cost of triplet formation and the infinite susceptibilities to spin dimerization might in this case translate in actual dimerization of the ground state.

Away from $n = 1$, the presence of a spin-valley “triplet” can also significantly affect the magnetic structure of the system. In particular, for systems which already exhibit ferromagnetism in the standard single-band Hubbard model, the inclusion of the spin-valley “triplet” can strengthen and extend the ferromagnetic phase. For example, generic 2 and 3 dimensional square lattice geometries, and others with similar connectivity conditions, exhibit Nagaoka ferromagnetism when the gain of kinetic energy of a single hole exceeds the decrease of superexchange energy. The latter condition is fulfilled at very large on-site interactions. In quantum dots in carbon nanotubes with small $\varepsilon$, Nagaoka-type ferromagnetism might become stable at reduced value of the interaction since the virtual hopping of the spin-valley triplets reduces the super-exchange penalty of having a polarized state.

For arrays with filling $1 < n < 2$ and zero detuning, the low energy physics consists of doubly and singly occupied dots while the occurrence of empty sites is strongly suppressed since it implies an increase of double occupancies. This implies that the number of electrons and doublons will be independently conserved and that the second term of $H_{ed}$ can be neglected. Also, the tunneling of the electrons and the doublons can be neglected. Thus, the only relevant terms in the effective Hamiltonian are the on-site energies, the long-range Coulomb and the electron-doublon exchange (second term in $H_{ed}$). This regime can lead to interesting phenomena when the electron-doublon exchange becomes comparable the multiplet splitting $\varepsilon$.

Finally, it should be pointed out that the long-range Coulomb interaction can have a preponderant influence in the charge distribution in small arrays of quantum dots.

### IV. SUMMARY AND CONCLUSIONS

We have presented a detailed study of the few-electron eigenspectrum of a double quantum dot in a semiconducting carbon nanotube. We showed how the spin-valley physics leads to the formation of multiplets. The internal energy structure of the multiplet is practically unaffected by a change in either the confinement potential or the interaction strength, but the energy gap between different multiplets is strongly modified by both. We showed that for sufficiently strong interactions, the spin-orbit coupling can exceed the energy splitting between states with symmetric and antisymmetric orbital parts for any detuning between the dots. This situation modifies the two particle phase diagram. Above a critical interaction strength, the ground state at small, finite magnetic fields is always ferromagnetic independent of the detuning. Furthermore, in this strongly interacting regime, the blockade of linear transport gradually disappears since the reduction of the multiplets’ energy splitting $\varepsilon$ allows a finite tunneling probability from the $|1L, 1R\rangle$ state to the $|2L, 0R\rangle$ state even for a symmetric spin-valley part. Pauli-blockade physics will occur for weak enough Coulomb correlations, which can be suppressed by either working with short dots, or by covering the nanotube by strong dielectric. We note that a well developed Pauli-blockade is the precondition for realization of spin-qubits in double dots allowing for coherent singlet-triplet manipulation.

Our understanding of the double dot physics can be used as an starting point to analyze the behavior of an array of coupled dots. The effective Hamiltonian, as presented in Eq. [31], can be applied to describe an array of coupled dots in certain regimes. In the future, we would like to explore the many-body physics associated with
the strong onsite correlations and its consequences in the
magnetic ordering of the system.
In the analysis presented here, we neglected terms that
flip either the spin or valley degree of freedom, or both.
However, such mechanisms could change the various level
crossings to avoided crossings and thus open new ways to
control the spin-valley degree of freedom as well as the
transport properties of this system.

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Appendix A: Coulomb matrix elements

We create an orthonormal set of localized single parti-
cle orbitals \( \Phi_i \), solving exactly the double dot system and
we use this set to construct the many-body Hamiltonian
for the interacting double-dot system:

\[
\hat{H} = \sum_i E_i \hat{a}_i^\dagger \hat{a}_i + \sum_{i\neq j} T_{ij} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{ijkl} U_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l.
\]  

(A1)

Here \( E_i = \langle \Phi_i | H_0 | \Phi_i \rangle \) are the single-particle energies,
\( T_{ij} = \langle \Phi_i | H_0 | \Phi_j \rangle \) are the tunneling matrix elements,
and \( U_{ijkl} = \langle \Phi_i | H_0 | \Phi_k \rangle \langle \Phi_j | H_0 | \Phi_l \rangle \)
correspond to the interaction matrix elements. At zero detuning,
the tunneling matrix elements, \( T_{ij} \), are only nonzero between states
with the same \( \sigma, \tau, n \) and located at different wells. For
nonzero detuning, tunneling between different bands becomes
possible. The electrons interact through the long-range Coulomb potential, Eq. [8] and the interaction matrix elements then take the form

\[
U_{nmpr} = \frac{e^2}{4\pi^2 k_d} \int \Phi_n^\dagger(\zeta_1) \cdot \Phi_p(\zeta_1) \Phi_m^\dagger(\zeta_2) \cdot \Phi_r(\zeta_2) \frac{1}{r} d\zeta_1 d\zeta_2 d\zeta_2,
\]  

(A2)

where

\[
\frac{1}{r} = \frac{1}{|r_1 - r_2|} = \frac{1}{\sqrt{2R^2[1 - \cos(\varphi_1 - \varphi_2)] + (\zeta_1 - \zeta_2)^2}}.
\]  

(A3)

To evaluate the interaction matrix elements, we use the following relation:

\[
\frac{1}{r} = \frac{1}{\pi} \int_{-\infty}^{\infty} e^{iq(\zeta_1 - \zeta_2)} K_0(R|2q\sin[(\varphi_1 - \varphi_2)/2]|) dq.
\]  

(A4)

If the rest of the integrand does not depend on \( \varphi_1 \) and \( \varphi_2 \),
the integration over those coordinates can be done analytically,

\[
\frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} K_0(R|2q\sin[(\varphi_1 - \varphi_2)/2]|) d\varphi_1 d\varphi_2 = I_0(R|q|) K_0(R|q|). \quad (A5)
\]

Also, the integration over \( \zeta_1 \) and \( \zeta_2 \) can be done analytically since \( \hat{F}(\zeta) \) has a simple functional dependence
that can be written in terms of exponentials with real or imaginary arguments. Once those integrals are obtained, we are left with the momentum integration over \( q \) in Eq. (A4). Defining

\[
F_{np}(q) = \int e^{iq\zeta_1} \{ \Phi_n^\dagger(\zeta_1) \Phi_p(\zeta_1) \} d\zeta_1, \quad (A6)
\]

we can write the Coulomb interaction matrix as a one-
dimensional numerical integration over the momentum \( q \).

\[
U_{nmpr} = \frac{e^2}{k_d \pi} \int F_{np}(q) F_{mr}(-q) I_0(R|q|) K_0(R|q|) dq. \quad (A7)
\]

In the calculation of the Coulomb matrix elements, we neglect
the dependence of the longitudinal wavevector \( k_n \) on spin, valley, and magnetic field. As discussed in Sec. II A, this approximation is good for \( \kappa \gg \Phi_{AB}/(\Phi_0 R), \Delta_{SO}/(2\hbar v) \), which is certainly true for the
parameters used in this paper.

There is another effective interaction that takes into
account intervalley scattering:

\[
U_{nmpr}^{KK'} = \frac{1}{4\pi^2} \int \Phi_n^\dagger(\zeta_1) \Phi_p(\zeta_1) \Phi_m^\dagger(\zeta_2) \Phi_r(\zeta_2) V^{KK'}(\varphi_1 \varphi_2 \zeta_1 \zeta_2) \quad (A8)
\]

where \( V^{KK'} \) is a short range interaction that can be taken
proportional to \( \delta(\zeta_1 - \zeta_2) \). We have estimate the \( U_{nmpr}^{KK'} \) terms and we have concluded that they only introduces
minor corrections. For that reason, we neglect this contribution
in the present work.

Appendix B: Rate equations

Here we derive the rate equations and the stationary
current corresponding the the setup depicted in Fig 10 a). At zero magnetic field and large detuning the single
particle ground state consists of the Kramer doublet \( |L1K \uparrow \rangle \) and \( |L1K \downarrow \rangle \) localized in the left dot. The two-
particle states are characterized by their charge degree of freedom and by their spin valley symmetry. The \( |2L, 0R \rangle \) and \( |1L, 1R \rangle \) states with antisymmetric spin-valley part
are non-degenerate and are called \( |M \rangle \) and \( |\bar{M} \rangle \) respectively. They are defined in Eq. (51) and (53). According
Due to the simple form of the $|1L,0R\rangle$ and $|1L,1R\rangle$ states with symmetric spin-valley part are each three fold degenerate and include the states $|FF\rangle$ and $|\tilde{F}F\rangle$ respectively. Following Eqs.(17) and (23) the structure of these states is given by:

$$|F_\pm\rangle = |FF\rangle = |2L,0R\rangle^+ |K\downarrow; K\uparrow\rangle$$
$$|F_0\rangle = |2L,0R\rangle^- |K\uparrow; K'\uparrow\rangle$$
$$|F_+\rangle = |2L,0R\rangle^- |K'\uparrow; K\uparrow\rangle$$
$$|\tilde{F}_-\rangle = |\tilde{F}F\rangle = |1L,1R\rangle^- |K\downarrow; K\downarrow\rangle$$
$$|\tilde{F}_0\rangle = |1L,1R\rangle^- |K\downarrow; K'\uparrow\rangle$$
$$|\tilde{F}_+\rangle = |1L,1R\rangle^- |K'\uparrow; K'\uparrow\rangle$$

Due to the serial setup each contact couples only to its adjacent dot. The tunneling rates to the collector (left contact in Fig.[10] (a)) depend on the correlated two particle states, which is accounted for by introducing the spectral weights $S_F$ and $S_M$ that determine how easy an electron tunneling between the left dot and the left reservoir can cause a transition between a two particle and one particle state on the dot.

$$S_F = \sum_m |\langle L1K\downarrow| a_{LMK_1} |F_-\rangle|^2$$
$$S_M = \sum_m |\langle L1K\downarrow| a_{LMK_1} |M\rangle|^2$$

Due to the simple form of the $|1L,1R\rangle$ wavefunctions the spectral weights corresponding to the tunneling between right contact and right dot has trivial spectral weights $S_M = |\langle L1K\downarrow| a_{LMK_1} |M\rangle|^2 = \frac{1}{2}$ and $S_F = |\langle L1K\downarrow| a_{LMK_1} |F_-\rangle|^2 = 1$.

We denote the reduced density matrix for the double dot by $P$ and denote off-diagonal matrix elements with $P_{ss'} := \langle s'|s\rangle = \langle P_{ss'} \rangle^*$, where $s$ and $s'$ are eigenstates of the double dot and diagonal elements with $P_s := \langle s|s\rangle$. We neglect processes that can mix states with different spin-valley part since hyperfine interaction is small in carbon nanotube and spin-orbit coupling is mainly a spin-valley coupling with a very weak effect on the longitudinal wave function. Then degenerate states are equally populated and the relevant matrix elements of the reduced density matrix for the double dot system are given by $P_1 = P_{L1K1\uparrow} + P_{L1L1\downarrow}$:

$$P_F = P_{F_+} + P_{F_0} + P_{F_-}; P_\tilde{F} = P_{\tilde{F}_+} + P_{\tilde{F}_0} + P_{\tilde{F}_-}, \text{ etc.}$$

The corresponding rate equations are given by:

$$d_t P_1 = -2\Gamma_E P_1 + \Gamma_C S_F P_F + 2\Gamma_C S_M P_M \quad (B1)$$
$$d_t P_F = -\Gamma_C S_F P_F - it_S(P_{\tilde{F}} - P_{\tilde{F}})$$
$$d_t P_{\tilde{F}} = \frac{3}{2} \Gamma_E P_1 + it_S(P_{\tilde{F}} - P_{\tilde{F}})$$
$$d_t P_{\tilde{F}} = -\frac{1}{2} \Gamma_C S_F + i\epsilon P_{\tilde{F}} - it_S(P_{\tilde{F}} - P_{\tilde{F}})$$
$$d_t P_M = -2\Gamma_C S_M P_M - it_S(P_{\tilde{M}} - P_{\tilde{M}})$$
$$d_t P_{\tilde{M}} = \frac{1}{2} \Gamma_E P_1 + it_S(P_{\tilde{M}} - P_{\tilde{M}})$$
$$d_t P_{\tilde{M}} = -\Gamma_C S_F P_{\tilde{F}} - it_S(P_{\tilde{M}} - P_{\tilde{M}})$$

with $P_1 + P_F + P_{\tilde{F}} + P_M + P_{\tilde{M}} = 1$. Here $\Gamma_E$ denotes the coupling strength to the emitter contact (right contact in Fig.[10] (a)) and $\Gamma_C$ denotes the coupling strength to the collector/ left contact.

These rate equations are solved analytically. The result for the stationary current and the occupation of the states are given by:

$$I_{on} = 2e\frac{\Gamma_E}{\hbar} P_1 = 2e\frac{\Gamma_E}{\hbar} 16S_F S_M t_{S}^2 t_{AS}^2 \Gamma_C / N \quad (B2)$$
$$P_{FF} = 3S_M t_{AS}^2 \Gamma_E (4t_{S}^2 + \Gamma_C^2 + \Gamma_R^2 + 4\epsilon^2)/N$$
$$N = 12S_M t_{AS}^2 \Gamma_E (2t_{S}^2 + \epsilon^2) + 3S_F S_M t_{AS}^2 \Gamma_C \Gamma_E + 2t_{S}^4 (4S_M t_{AS}^2 \Gamma_C + 2t_{AS} \Gamma_E + S_M t_{AS} \Gamma_E)$$

Here $t_{AS}$ denotes the interdot tunneling between states $|M\rangle$ and $|\tilde{M}\rangle$ and $t_s$ the interdot tunneling between the states $|FF\rangle$ and $|\tilde{F}F\rangle$. Spectral weights $S_F$ and $S_M$ account for the overlap between an electron hopping onto the dot and the two particle eigenstates, and $\Gamma_C$ and $\Gamma_E$ are the coupling strength to emitter and collector.

The stationary current $I_{on}$ vanishes as $1/e^2$ for large $\epsilon$. We note that for reversed transport voltage still a finite current can pass through the double dot, so that for large $\epsilon$ the double dot acts as a current rectifier. We calculate the current for the unblocked voltage direction. Inverting the bias voltage depicted in Fig.[10] (a) current flows by electrons hopping from the left reservoir through the double dot to the right reservoir. Applying again the rate equation approach and obtain:

$$I_{off} = 2e\frac{\Gamma_R}{\hbar} P_1 = 2e\frac{\Gamma_R^2 t_{AS}^2}{\hbar^2 t_{AS}^2 (\Gamma_R + 2S_M \Gamma_L)} + S_M \Gamma_L \Gamma_R (B3)$$

We note that $\Gamma_L$ corresponds to $\Gamma_C$ in Eq. (B2) and $\Gamma_R$ corresponds to $\Gamma_E$. 