Recent studies reveal that a double-quantum-dot system hosting more than two electrons may be superior in certain aspects as compared to the traditional case in which only two electrons are confined (a singlet–triplet qubit). The electron–phonon dephasing occurring in a GaAs multi-electron double-quantum-dot system is studied, in a biased case in which the singlet state is hybridized, as well as in an unbiased case in which the hybridization is absent. It is found that while the electron–phonon dephasing rate increases with the number of electrons confined in the unbiased case, this does not hold in the biased case. A merit figure is defined as a ratio between the exchange energy and the dephasing rate, and have shown that in experimentally relevant range of the exchange energy, the merit figure actually increases with the number of electrons in the biased case. The results show that the multi-electron quantum-dots system has another advantage in mitigating the effect of electron–phonon dephasing, which is previously under-appreciated in the literature.

1. Introduction

Semiconductor quantum-dot spin qubits as platforms for the physical realization of quantum computation, have attracted extensive research interests due to their promises of tunability, scalability and high-fidelity gate operations[1–26] While each quantum dot typically hosts no more than two electrons in traditional spin qubits, recent researches reveal that the multi-electron qubits, in which certain dot is allowed to host more than two electrons, may be advantageous in some aspects.[27–44] For example, a multi-electron quantum dot may serve as a mediator for fast spin exchange[27] or a tunable coupling between nearby dots.[13] Moreover, it has been shown that multi-electron quantum-dot devices may be more resilient to noises than traditional ones due to the screening effect by core electrons.[40–42]

Experiments show that in certain asymmetric multi-electron triple-quantum-dot system, the dependence of the exchange energy on the absolute value of detuning can be non-monotonic, implying the existence of a sweet spot.[37] It has also been observed in a similar system that the sign of the exchange energy may reverse, removing a long-standing constraint for the construction of dynamically corrected exchange gates.[38] On the theory side, calculations based on the configuration interaction (CI) techniques on few-electron multi-quantum-dot systems have demonstrated negative exchange interactions and their implication on robust quantum control.[44–46] Other studies on these systems have unveiled their potentials for tunable couplings,[42] robust quantum gates,[42] as well as other interesting properties.[43] These results have shown the promises of multi-electron quantum-dot systems in achieving noise-resilient quantum information processing.

Various environmental noises and ways to combat them have been extensively studied in conventional two-electron singlet–triplet qubits.[47–70] Among these noises, the electron–phonon dephasing is an important channel leading to decoherence.[47–51] Phonon couplings that contribute to decoherence in GaAs include the deformation potential interaction, the polar optical interaction, and the piezoelectric interaction.[59] In double quantum dots (DQD) hosting two electrons, it has been shown that the deformation potential and piezoelectric interaction play major roles in the electron–phonon dephasing, and all channels of phonon couplings reduce as the dot distance increases.[49,50] It is an interesting open question how the behavior of the electron–phonon dephasing may change as the number of electrons in the DQD is increased.[46]

In this paper, we investigate the electron–phonon dephasing in a GaAs multi-electron DQD system, in which the electron configurations, the definition of singlet and triplet, and their hybridization are more complicated than the case with only two electrons. In this work, we consider phonon-mediated dephasing in two cases: the unbiased case and the biased case. In the unbiased case, the hybridization between lowest singlet states is minimized. In the biased case, the hybridization is enhanced since the first excited singlet states are energetically brought closer to the lowest singlet state by a larger relative detuning between two dots in a DQD. We have defined a merit figure as a ratio between the exchange energy and the dephasing rate in biased case, and have shown that in experimentally relevant range of the exchange energy, the merit figure actually increases with the number of electrons. These results suggest that the multi-electron...
quantum-dot systems have advantages in reducing noises stemming from the electron–phonon interaction, which is previously under-appreciated in the literature.

The remainder of the paper is organized as follows. In Section 2 we present our model of the multi-electron DQD system, and methods to solve the electron–phonon interaction problem. Section 3 shows the results on the dephasing rates, exchange energies and the merit figures in different cases. In the end we conclude in Section 4.

2. Model and Methods

2.1. Hamiltonian

Here we consider an asymmetric double-quantum-dot system where the right dot (R) is larger than the left dot (L), and the distance between the center of the two dots is 2x₀. We keep the lowest N orbitals in the right dot and label the energy levels from the ground state to the Nth orbital by R₁ through Rₙ as shown in Figure 1. We assume that the system hosts a total of 2N electrons with one electron in the left dot (L) and 2N − 1 electrons in the right dot (R). The Hamiltonian of the system can be written as

\[ H_{e} = \sum_{j} E_j a_j^\dagger a_j + \sum_{j,k} e \left| R_j - R_k \right| \]

where

\[ e = \frac{-i \hbar \nabla_j + eA_j}{2m^*} + V(r) + g^* \mu_B \mathbf{B} \cdot \mathbf{S} \]  

The confinement potential in the xy plane is

\[ V(r) = \frac{1}{2} m^* \text{Min} \left[ \omega_0^2 \left( r - r_0 \right)^2 - \Delta, \omega_0^2 \left| r + r_0 \right|^2 + \Delta \right] \]

where \( \omega_0 \) (\( \omega_p \)) is the confinement strength in dot L (R), \( r = (x, y) \), \( r_0 = (x_0, 0) \), \( x_0 \) is half the distance between the center of the two dots, \( m^* = 0.067m_e \) is the effective mass of the electron, and \( \Delta \) is the detuning, as indicated in Figure 1. Last term of \( h_e \) is Zeeman energy of the electrons, \( g^* \) is g-factor value of electron, \( \mu_B \) is bohr magneton, \( \mathbf{B} = B \hat{z} \) is the perpendicular magnetic field and \( \mathbf{S} \) is the total electron spin, the magnetic field is set at \( B = 0.7T \). In our model, \( \hbar \omega_L > \hbar \omega_R \), \( \hbar \omega_L = 2.838 \text{ meV} \), \( \hbar \omega_R \) vary between \( \hbar \omega_L / 4 \) and \( \hbar \omega_L / 2 \).

We consider a singlet–triplet (ST) qubit realized in the detuning regime where the electron occupancy is \( (n_L, n_R) \approx (1, 2N - 1) \). We use the notation \( (n_L, n_R) \) to indicate the number of electrons in the left \( n_L \) and right \( n_R \) dots. We denote a singlet (triplet) formed by \( n_r \) electrons in the left dot and \( n_n \) electrons in the right dot as \( |S(n_L, n_R)\rangle \) (\( |T(n_L, n_R)\rangle \)). In this work, we study the dephasing for two cases: 1) The logical bases are \( |S(1, 2N - 1)\rangle \) and \( |T(1, 2N - 1)\rangle \). We refer this as an “unbiased” case. 2) The logical bases are a hybridized singlet \( |S(0, 2N)\rangle / |S(2, 2N - 2)\rangle \) and \( |T(1, 2N - 1)\rangle \). We refer this as a “biased” case. For the biased case, the hybridized singlet depends on the direction of the detuning \( \Delta \). For a large positive detuning, the hybridized singlet is \( |S_{\text{mix}}^{(0,2N)}\rangle \). On the other hand, for a small positive detuning or a negative detuning, the hybridized singlet is \( |S_{\text{mix}}^{(2N-2)}\rangle \).

In biased case, the exchange energy between singlet and triplet states is a key quantity in our discussion. To evaluate the exchange energy as a function of detuning, we consider an effective Hamiltonian written in the bases of \( |S(1, 2N - 1)\rangle \), \( |T(1, 2N - 1)\rangle \) and \( |S(0, 2N)\rangle \) for the large positive detuning regime while \( |S(1, 2N - 1)\rangle \), \( |T(1, 2N - 1)\rangle \), and \( |S(2, 2N - 2)\rangle \) for the small positive or negative detuning regime. We have confirmed that other electron configurations exhibit much larger energy and, therefore, they do not affect the exchange energy in any important way (see Appendix A). Diagonalizing the effective Hamiltonian, the exchange energy is

\[ J = E_{S} - E_{T} \]

where \( |S\rangle \) and \( |T\rangle \) are the lowest singlet and triplet states respectively, \( E_{S} \), \( E_{T} \) are their eigenvalues of Hamiltonian.

2.2. Singlet and Triplet in Multi-Electron Double Quantum Dot

Similar to two-electron case, singlet–triplet spin qubits in multi-electron DQD can also be well defined. In the unbiased case, the singlet state is \( |S(1, 2N - 1)\rangle \) and the triplet state is \( |T(1, 2N - 1)\rangle \) can be written as

\[ |S(1, 2N - 1)\rangle = \frac{1}{\sqrt{2(1 + I_{R})}} \left( \uparrow_{R_1} \downarrow_{R_2} + \uparrow_{L_1} \downarrow_{L_2} \right) \]


\[ |T(1, 2N - 1)| = \frac{1}{\sqrt{2(1 - I_{N,T})}} (|r_L, r_R| - |r_R, r_L|) \]  
\[ \text{where} \]
\[ |r_L, r_R| = |l_{R_1}, r_{R_1}, r_{R_1}, \ldots, r_{R_i}, l_{R_{i+1}}\rangle \]
\[ |r_R, l_R| = |r_{R_1}, r_{R_1}, l_{R_1}, \ldots, l_{R_i}, r_{R_{i+1}}\rangle \]
are 2N-electron slater determinant with different electron configuration in DQD, \( L_1 \) and \( R_i \) (\( i = 1 \ldots N \)) label the orbital states occupied by electrons in the left and right dots as shown in Figure 1. \( \uparrow \) and \( \downarrow \) represents spins, and \( I_{N,S} \) and \( I_{N,T} \) are factors related to normalization, given in Appendix B. Therefore the singlet is symmetric while the triplet is anti-symmetric in multi-electron case as we defined. When \( N = 1 \), we have a conventional two-electron ST qubit.\(^{[50]}\)

In the biased DQD, due to different detuning values, the singlet states hybridize as a combination of Slater determinants. For a large positive detuning, the singlet is hybridized as
\[
|S^{(2N)}_{\text{max}}\rangle = \frac{|S(1, 2N - 1) + \beta |S(0, 2N)|}{\sqrt{1 + \beta^2}}
\]

or for a small positive detuning or a negative detuning, the hybridized singlet is
\[
|S^{(2N-2)}_{\text{max}}\rangle = \frac{|S(1, 2N - 1) + \beta |S(2, 2N - 2)|}{\sqrt{1 + \beta^2}}
\]

\[ 1/\sqrt{1 + \beta^2} \text{ and } \beta/\sqrt{1 + \beta^2} \text{ are both functions of detuning, and} \]
\[ |S(0, 2N)\rangle = \sum_l |r_{R_1}, l_{L_1}\rangle \]
\[ |S(2, 2N - 2)\rangle = \sum_l |l_{R_1}, r_{L_1}\rangle \]
\[ |S(1, 2N - 1)\rangle = \sum_l |r_{R_1}, r_{R_1}, r_{R_1}, \ldots, r_{R_i}, l_{R_{i+1}}\rangle \]
\[ |r_{R_1}, r_{R_1}, l_{R_1}, \ldots, l_{R_i}, r_{R_{i+1}}\rangle \]

are also Slater determinant with electron configuration we considered in this work.

### 2.3. Multi-Electron Dephasing of Electron–Phonon Interaction

The total Hamiltonian is\(^{[71]}\)
\[ H = H_e + H_{ph} + H_{ep} \]  
\[ \text{where} \]
\[ H_e \] is the system Hamiltonian of electrons in a DQD (Equation (1)). \( H_{ph} = \sum_{q \neq 0} a_{q \downarrow} a_{q \uparrow} \) is the environment Hamiltonian described by phonon modes, and \( H_{ep} \) is the electron–phonon interaction.

For a singlet–triplet qubit, \( H_e \) is written in the bases of the lowest singlet, \( |S\rangle \), and lowest triplet state, \( |T\rangle \), that is
\[ H_e = \frac{1}{2} \sigma_z \]
\[ \text{where} \]
\[ \sigma_z = |T\rangle\langle T| - |S\rangle\langle S| \] (see Section 2.2 for details).

In a semiconductor, \( H_{ep} \) is the Hamiltonian that describes effective electron–phonon interaction takes the form\(^{[50]}\)
\[ H_{ep} = \sum_{m \neq 0} |m\rangle \rho(q) |a_{m \downarrow} + a_{m \uparrow}\rangle \]

where \( a_{m \downarrow} \) and \( a_{m \uparrow}^\dagger \) are phonon annihilation and creation operators respectively, \( q \) the lattice momentum, and \( \lambda \) the branch index, \( \rho(q) \) is the electron density operator, taking the form \( \rho(q) = \sum_{m \neq 0} e^{i \mathbf{q} \cdot \mathbf{R}} \) in 2N electron DQD system. \( M(q) \) represents different kinds of electron–phonon interactions. In GaAs DQD, the deformation potential (DP) and piezoelectric (PE) interaction provides the main contribution to the phonon dephasing, while contributions from other interactions are negligible.\(^{[45,50]}\) The DP and PE have the form\(^{[50]}\)
\[ M_{\text{DP}}^{\text{GaAs}}(q) = D \left( \frac{h}{\rho v_{\text{ph}}} \right) \frac{i}{2} |q| \]
\[ M_{\text{PE}}^{\text{GaAs}}(q) = i \left( \frac{h}{\rho v_{\text{ph}}} \right) 2 e \epsilon_{ee} (q) \times |q| \]

\[ \text{and one should note that } M_{\text{DP}}^{\text{GaAs}}(q) \text{ only couples electrons to longitudinal acoustic phonons and } M_{\text{PE}}^{\text{GaAs}}(q) \text{ can couple electrons to both LA and transverse acoustic phonons. Here, } D = 8.66 \text{ eV} \text{ is the deformation constant, } \rho = 5.3 \times 10^3 \text{ kg m}^{-3} \text{ the mass density, } e \text{ is elementary electric charge, } \epsilon_{ee} = 1.38 \times 10^9 \text{ V m}^{-1} \text{ is elasticity tensor component, } \xi \text{ is the polarization vector, and } \omega_q \text{ the angular frequency of the phonon mode } q. \text{ We further define } \gamma_v \text{ as the population relaxation rate of the phonon mode } q, \text{ which is assumed to have the form } \gamma_v = y_v \omega_q^{5/2} \text{ in our calculations. We fix } y_v = 10^9 \text{ Hz and consider cases in which } n = 2 \text{ or } n = 3 \text{ and have also verified that other values of } y_v \text{ and } n \text{ will not significantly change our main findings.} \]

For a two-level system (a qubit system), the off-diagonal element of the effective electron–phonon interaction Hamiltonian leads to a decay in the form\(^{[72,73]}\)
\[ \rho_{ST}(t) = \rho_{ST}(0) e^{-B^2(t)} \]

where \( B^2(t) \) is dephasing factor. For a singlet–triplet qubit realized in 2N-electron system, the logical eigenstates are defined as the lowest singlet and triplet states. Written in the bases of \( |S\rangle \) and \( |T\rangle \)
\[ H_{ep} = \left( \frac{|T\rangle\langle H_{ep}|T\rangle}{\langle T|H_{ep}|T\rangle} \langle T|H_{ep}|S\rangle \right) |S\rangle |H_{ep}|S\rangle + \langle T|H_{ep}|T\rangle |T\rangle |H_{ep}|T\rangle / 2, \text{ since } H_{ep} \text{ has no spin dependence} \]
and imaginary part, $H_{ep}$ and $H_{ep}'$ are zero. Therefore we can rewrite $H_{ep}$ as

$$H_{ep} = \sum_{q,\omega} M_{q}(\omega) A_{q} \sigma_{z} (a_{q,\omega} + a_{q,\omega}^{\dagger})$$

(23)

where $A_{q}$ is

$$A_{q} = \frac{1}{2} \{ [T] \rho(q) | T \} - \langle S | \rho(q) | S \rangle$$

(24)

see Appendix B for details.

For a dissipative phonon reservoir with finite $\gamma_{q}$, the main contribution to $B^2(t)$ can be calculated by \cite{50,72}

$$B^2_{\text{Decay}}(t) = \frac{V}{2 \pi^3 \hbar^2} \int d^3q \frac{|M(q) A_{q}(q)|^2 \gamma_{q}}{\omega_{q}^2 + \gamma_{q}^2/4} \lesssim \Gamma_{ST}$$

(25)

where $\Gamma_{ST}$, the dephasing rate, is the key quantity considered in this paper.

3. Results

3.1. Dephasing Rate of Unbiased Case

According to Equation (25), the electron–phonon dephasing rate can be expressed as

$$\Gamma_{ST} = \frac{V}{2 \pi^3 \hbar^2} \int d^3q \frac{|M(q) A_{q}(q)|^2 \gamma_{q}}{\omega_{q}^2 + \gamma_{q}^2/4}$$

(26)

In the unbiased case, $A_{q}$ is dependent on the singlet state Equation (5) and triplet state Equation (6), suggesting that $\Gamma_{ST}$ varies with the number of electrons.

Here we consider three unbiased cases with electron configurations (1,1), (1,3), and (1,7) with the first entry showing the number of electron in dot L and the second dot R. A schematic showing the latter two cases is shown in Figure 1b. Details on the evaluation of $A_{q}$ in these cases are given in Appendix B.

Figure 2 shows the dephasing rate $\Gamma_{ST}$ as functions of the half dot distance $x_0$ with different confinement strength $h\omega_{q}$ as indicated. The three values of the confinement strength on dot R $h\omega_{q} = 1.419$, 0.946, and 0.709 meV correspond to dot sizes 28.076, 33.981, and 38.627 nm, respectively. Several features can be clearly seen from the figure. First, the dephasing rate rapidly decreases with increasing $x_0$ in all cases. The results for (1,1) are consistent with ref. [50], and it is not surprising that results for (1,3) and (1,7) are similar. Second, for a given confinement strength, the dephasing rate is greatest for (1,7) as more electrons imply larger integration from $A_{q}$ as Appendix B shows, implying more channels of electron–phonon interaction. Similarly, the effect is intermediate for (1,3), and smallest for (1,1). Third, when $x_0$ and $h\omega_{q}$ are fixed, the dephasing rate is greater when dot R is larger (smaller $h\omega_{q}$) and smaller when dot R is smaller (larger $h\omega_{q}$). As can be seen from Equation (B12), the behavior of $A_{q}$ is controlled by integrals Equations (B15), (B16), and (B17), for the cases of (1,1), (1,3), and (1,7), respectively. The l.h.s. of Equations (B15)–(B17) decreases either as $x_0$ increase, or as dots get smaller.

3.2. Biased Case and the Merit Figure

As the detuning $\Delta$ changes, the singlet states start to hybridize as suggested by Equation (9) or (10). Figure 3 shows the dephasing rate $\Gamma_{ST}$ as functions of $\beta/\sqrt{1 + \beta^2}$ for six different hybridized states as indicated (the normalization constant is ignored in the legend). Note that for small $\beta$, what we call the hybridization ratio $\beta/\sqrt{1 + \beta^2} \approx \beta$ indicates the ratio of the hybridization to states other than the (1,1), (1,3), and (1,7) states considered. Figure 3a shows the range $0 < \beta/\sqrt{1 + \beta^2} < 0.05$ while Figure 3b the range $0.05 < \beta/\sqrt{1 + \beta^2} < 0.10$. We can see that while $\Gamma_{ST}$ increases monotonically with the hybridization ratio, the order of the results for states with mainly (1,1), (1,3), and (1,7) character changes. In particular, for $\beta/\sqrt{1 + \beta^2} = 0$ the dephasing rate for the state (1,1) is the smallest, consistent with the unbiased case. However, for $\beta/\sqrt{1 + \beta^2} \geq 0.02$ the dephasing rate for the state with mainly (1,1) character becomes the largest, which is greater than the case with mainly (1,3) character by about 30% and the case with mainly (1,7) character by about 60% at $\beta/\sqrt{1 + \beta^2} \approx 0.1$, as can be seen from the inset of Figure 3b. This result is opposite to the unbiased case and is a direct consequence of the state hybridization, as described in the following paragraph and Appendix B.

The numerical results in Figure 3b can be understood by inspecting the explicit forms of $\Gamma_{ST}$ [Equation (26)], $A_{q}$ [Equation (B18)], and the electron density of the fully occupied sin-
...glet state, $\langle S(0, 2N)|\rho(q)|S(0, 2N)\rangle$ [Equation (B20)]. Since $\Gamma_{ST}$ depends on the magnitude of $|A_q|$ [Equation (26)], at a fixed value of hybridization, $\beta/\sqrt{1 + \beta^2}$, Equation (B18) suggests that the magnitudes of $A_q$ for different numbers of electrons depend on the magnitude of $\langle S(0, 2N)|\rho(q)|S(0, 2N)\rangle$. Alternatively, the reduction of dephasing for a larger number of electrons can be understood by examining the magnitudes $|A_q|$ at the limit where $\beta/\sqrt{1 + \beta^2} \approx 1$. In that limit, mathematically, the additional nodes of the excited orbitals lead to extra terms with negative coefficients in the expression of $|A_q|$, which in turn result in a smaller magnitude of $|A_q|$. Physically, we could interpret that the reduction of dephasing results from the oscillations of the excited wavefunctions in the position space, which interfere destructively with the fluctuations by the deformation potential. Therefore, the above analysis leads to the conclusion that the physical point of view of the decrease in the dephasing rate with the number of electrons can be attributed to the larger electron density of the fully occupied singlet state, $\langle S(0, 2N)|\rho(q)|S(0, 2N)\rangle$. The argument above can be similarly applied on the biased case in which the $|S(1, 2N - 1)\rangle$ hybridizes with $|S(2, 2N - 2)\rangle$ [Equations (B19) and (B21)].

**Figure 4** shows the hybridization ratio $\beta/\sqrt{1 + \beta^2}$ versus the exchange interaction $J$ as calculated from Equation (4). In general, the more hybridized the singlet state is, the larger the absolute value of detuning should be, and as a consequence, the greater the value of $J$ is. For the same value of $J$, the state with mainly $(1,1)$ character has a greater hybridization ratio.$^{[74]}$

To reveal the performance of our system in realistic situations, we define the merit $M = J/\hbar \Gamma_{ST}$ as the ratio between the exchange gate time given by $\hbar/J$ and the decay time given by $1/\Gamma_{ST}$. The definition of merit $M$ assumes the negative role of electron–phonon interaction on the coherence of the logical states, as suggested by the conformity between the theoretical work$^{[80]}$ and the experimental work$^{[82]}$ on the decoherence rate of a two-electron singlet–triplet qubit in a DQD device. This is in contrast to other works which show that the dissipation effect serves to enhance the stability of quantum system.$^{[76–79]}$ In particular, ref. $^{[80]}$ has demonstrated, by applying a periodical driving, that the stability of a quantum metastable system is enhanced. However, investigating the positive role of electron–phonon interaction in the coherence of a multielectron singlet–triplet qubit is currently out of scope of this work.

The results of the merit $M$ as functions of the exchange energy is shown in **Figure 5**, which is the key result of this paper. The non-monotonic behavior of the $M$ versus $J$ curves shown in Figure 5 is a combinational effect of the changing rate of $\Gamma_{ST}$...
and $J$ as functions of $\beta/\sqrt{1+\beta^2}$. More importantly, the merit figure for states associated with $(1,3)$ and $(1,7)$ are greater than those associated with $(1,1)$. This indicates that multi-electron quantum dots may offer advantages in electron–phonon dephasing, which is the main result of this paper. The results shown in Figure 5 is divided into two regions: $J < 0.04$ meV (marked by yellow), and $J \geq 0.04$ meV (marked by cyan). In the right (cyan) region, the merit figures for states associated with $(1,7)$ are greater than those for $(1,3)$, while the merit figure for the state with $(1,1)$ is the smallest. Given the fact that in practical operations of the qubit, the exchange interaction should neither be too small nor too large. Therefore, in the regime of $J \geq 0.04$ meV, having more electrons in the right dot implies a better merit figure, which is advantageous in experiments. This is the key finding of this paper. We have also verified that our conclusion holds for other experimentally relevant parameters, including the dot distance and dot sizes (confinement strength), and selective results are shown in Appendix C. This behavior is understandable from Figures 3 and 4. From Figure 4, one sees that at a fixed value of $\beta/\sqrt{1+\beta^2}$, $J$ is the largest for states associated with $(1,7)$, intermediate for $(1,3)$ and smallest for $(1,1)$, and the differences between them are quite appreciable. On the other hand, from Figure 3 one sees that for the same value of $\beta/\sqrt{1+\beta^2}$, the values of $\Gamma_{ST}$ are close. Since $J$ is on the numerator of the merit figure, the merit figure should follow the same trend as observed in Figure 4.

Since, as discussed in the previous paragraph, the behavior of the merit figure follows the behavior of $J$, the critical value $J = 0.04$ meV can be understood from the relationship between the number of electrons and the magnitude of $J$. For the regime in which $J > 0.04$ meV and a larger number of electrons, at a larger value of hybridization $\beta/\sqrt{V^2 + 1}$, since the wavefunctions of the excited orbitals are more extended in space, the enhanced overlap between wavefunctions in the left and right dots results in larger exchange energy. On the other hand, for the regime in which $J < 0.04$ meV, at a small value of hybridization $\beta/\sqrt{V^2 + 1}$, the overlap only occurs near the very end of the tails of the valence orbitals, which exhibit similar forms for a four- and eight-electron singlet–triplet qubit. This results in a comparable magnitude of $J$ for a four- and eight-electron singlet–triplet qubit.

### 4. Conclusions

In this paper, we have calculated the dephasing rate, exchange energy, and the merit figure of a multi-electron quantum-dot system with one electron in the left dot and 1, 3, or 7 electrons in the right dot. We have found that in the unbiased case, the dephasing rate in general increases with the number of electrons in the right dot. This is however not necessarily true in the biased case. Nevertheless, as we have shown that in the experimentally relevant regime $J \geq 0.04$ meV, having more electrons in the right dot implies a better merit figure. Our results suggest that multi-electron quantum dots may be advantageous in certain cases.

**Appendix A: System Hamiltonian and Exchange Energy**

In 2N-electron system, the effective Hamiltonian can be written in extended Hubbard model\(^{73,81}\):

$$H_e = \sum_{j,\sigma} \varepsilon_{j,\sigma} c_{j,\sigma}^\dagger c_{j,\sigma} + \sum_{j<k} U_{j,k} n_{j,\sigma} n_{k,\sigma} + \sum_{j<k} \sum_{\sigma} U_{j,k} e_{j,\sigma}^c e_{k,\sigma}^c + H.c.$$

where

$$U_{j,k} = \int \Psi^*_j(r_2) \Psi^*_k(r_1) C(r_1, r_2) \Psi_j(r_1) \Psi_k(r_1) \, dr_2^2$$

and $U_{j,k}$ is the on-site Coulomb interaction, $C(r_1, r_2)$ is the hopping integral, $\Psi_j(r_1)$ and $\Psi_k(r_1)$ are orbitals, and $\varepsilon_{j,\sigma}$ is the on-site energy at $j$. In the unbiased case, the hopping integral $C(r_1, r_2)$ is the direct exchange Coulomb interaction between the $j$th orbital and $k$th orbital.

We denote 2N-electron Slater determinants as

$$|S(t_{11}, t_{12}, \ldots, t_{N1}, t_{N2}, \ldots)|$$

where

$$t_{11} = 1 \quad t_{12} = 1 \quad \ldots \quad t_{N1} = 1 \quad t_{N2} = 1$$

are 2N-electron Slater determinants, here $m \geq N$. Normalization coefficients are dropped for simplicity.

We can write effective Hubbard Hamiltonian of four-electron in the bases: $|S(t_{11}, t_{12})\rangle$, $|T(t_{11}, t_{12})\rangle$, $|S(t_{11}, t_{12})\rangle$, $|T(t_{11}, t_{12})\rangle$, $|S(t_{11}, t_{12})\rangle$, $|T(t_{11}, t_{12})\rangle$. With 2$e_{R_1}$ energy shift, diagonal elements of system Hamiltonian are

$$\text{diag}(|S(t_{11}, t_{12})\rangle) = \varepsilon_{11} + \varepsilon_{22} + U_{R_1} + 2U_{R_1, R_2} + 2U_{R_1, R_2} - U_{R_1, R_2}$$

$$- U_{R_1, R_2}$$

$$\text{diag}(|T(t_{11}, t_{12})\rangle) = \varepsilon_{11} + \varepsilon_{22} + U_{R_1} + 2U_{R_1, R_2} + 2U_{R_1, R_2} - U_{R_1, R_2}$$

$$- U_{R_1, R_2}$$

$$\text{diag}(|S(t_{11}, t_{12})\rangle) = \varepsilon_{11} + \varepsilon_{22} + U_{R_1} + 2U_{R_1, R_2} + 2U_{R_1, R_2} - U_{R_1, R_2}$$

$$- U_{R_1, R_2}$$

$$\text{diag}(|T(t_{11}, t_{12})\rangle) = \varepsilon_{11} + \varepsilon_{22} + U_{R_1} + 2U_{R_1, R_2} + 2U_{R_1, R_2} - U_{R_1, R_2}$$

$$- U_{R_1, R_2}$$
For eight-electron effective Hubbard Hamiltonian can be written in bases of \( \{ \ket{S(\uparrow_1 \uparrow_2 \downarrow_1 \downarrow_2)}, \ket{IT(\downarrow_1 \uparrow_2 \downarrow_2)}, \ket{IT(\uparrow_1 \downarrow_2)}, \ket{IS(\uparrow_1 \downarrow_1 \downarrow_2)}, \ket{IT(\uparrow_1 \downarrow_1)}, \ket{IS(\uparrow_1 \downarrow_2 \downarrow_1)}, \ket{IS(\uparrow_1 \downarrow_1 \uparrow_2)}, \ket{IS(\uparrow_1 \downarrow_1 \downarrow_1) \} \}\), with energy shift of \( 2 \varepsilon_{R_1} + 2 \varepsilon_{R_2} + 2 \varepsilon_{L_1} \), diagonal elements are:

\[
\text{diag}(\{S(\uparrow_1 \uparrow_2 \downarrow_1 \downarrow_2)\}) = \varepsilon_{R_1} + \varepsilon_{R_2} + \varepsilon_{L_1} + 2U_{R_1,R_2} + 2U_{R_1,R_3} + 2U_{R_1,R_4} + 2U_{R_2,R_3} + 2U_{R_2,R_4} - U^e_{R_1,R_2} - U^e_{R_1,R_3} - U^e_{R_1,R_4} - U^e_{R_2,R_3} - U^e_{R_2,R_4} - U^e_{R_3,R_4} (A20)
\]

\[
\text{diag}(\{T(\downarrow_1 \uparrow_2 \downarrow_2)\}) = \varepsilon_{R_1} + \varepsilon_{R_2} + \varepsilon_{L_1} + 2U_{R_1,R_2} + 2U_{R_1,R_3} + 2U_{R_2,R_3} + 2U_{R_2,R_4} - U^e_{R_1,R_2} - U^e_{R_1,R_3} - U^e_{R_1,R_4} - U^e_{R_2,R_3} - U^e_{R_2,R_4} - U^e_{R_3,R_4} (A21)
\]

\[
\text{diag}(\{S(\uparrow_1 \downarrow_2 \downarrow_1 \downarrow_2)\}) = 2\varepsilon_{R_1} + \varepsilon_{R_2} + \varepsilon_{L_1} + 4U_{R_1,R_2} - 2U^e_{R_1,R_2} - 2U^e_{R_1,R_3} - 2U^e_{R_1,R_4} - 2U^e_{R_2,R_3} - 2U^e_{R_2,R_4} - 2U^e_{R_3,R_4} (A22)
\]

\[
\text{diag}(\{T(\uparrow_1 \downarrow_1 \downarrow_2)\}) = \varepsilon_{R_1} + \varepsilon_{R_2} + \varepsilon_{L_1} + 2U_{R_1,R_2} + 2U_{R_1,R_3} + 2U_{R_1,R_4} + 2U_{R_2,R_3} + 2U_{R_2,R_4} - U^e_{R_1,R_2} - U^e_{R_1,R_3} - U^e_{R_1,R_4} - U^e_{R_2,R_3} - U^e_{R_2,R_4} - U^e_{R_3,R_4} (A23)
\]

\[
\text{diag}(\{T(\downarrow_1 \uparrow_2)\}) = \varepsilon_{R_1} + \varepsilon_{R_2} + \varepsilon_{L_1} + 2U_{R_1,R_2} + 2U_{R_1,R_3} + 2U_{R_1,R_4} + 2U_{R_2,R_3} + 2U_{R_2,R_4} - U^e_{R_1,R_2} - U^e_{R_1,R_3} - U^e_{R_1,R_4} - U^e_{R_2,R_3} - U^e_{R_2,R_4} - U^e_{R_3,R_4} (A24)
\]

\[
\text{diag}(\{S(\uparrow_1 \downarrow_1)\}) = \varepsilon_{R_1} + \varepsilon_{R_2} + \varepsilon_{L_1} + 2U_{R_1,R_2} + 2U_{R_1,R_3} + 2U_{R_1,R_4} + 2U_{R_2,R_3} + 2U_{R_2,R_4} - U^e_{R_1,R_2} - U^e_{R_1,R_3} - U^e_{R_1,R_4} - U^e_{R_2,R_3} - U^e_{R_2,R_4} - U^e_{R_3,R_4} (A25)
\]

\[
\text{diag}(\{T(\downarrow_1 \uparrow_2 \downarrow_2)\}) = \varepsilon_{R_1} + \varepsilon_{R_2} + \varepsilon_{L_1} + 2U_{R_1,R_2} + 2U_{R_1,R_3} + 2U_{R_1,R_4} + 2U_{R_2,R_3} + 2U_{R_2,R_4} - U^e_{R_1,R_2} - U^e_{R_1,R_3} - U^e_{R_1,R_4} - U^e_{R_2,R_3} - U^e_{R_2,R_4} - U^e_{R_3,R_4} (A26)
\]
therefore we can obtain

\[ | \Psi \rangle = \frac{1}{\sqrt{2}} (| \uparrow \downarrow \rangle + | \downarrow \uparrow \rangle) \]

where \( | \Psi \rangle \) is the eigenstate of the Hamiltonian.

In the unbiased case, the singlet and triplet states can be written

\[ | S \rangle = | \uparrow \uparrow \rangle - | \downarrow \downarrow \rangle \]
\[ | T \rangle = | \uparrow \downarrow \rangle + | \downarrow \uparrow \rangle \]

and

\[ | T \rangle = | \uparrow \downarrow \rangle + | \downarrow \uparrow \rangle \]

where \(|S\rangle\) and \(|T\rangle\) satisfy

\[ \langle S | S \rangle = 1, \langle T | T \rangle = 1, \langle S | T \rangle = 0 \]

therefore we can obtain

\[ a = \frac{1}{\sqrt{2(1 + I_{N,S})}}, \quad b = \frac{1}{\sqrt{2(1 - I_{N,T})}} \]

as indicated in Equations (5) and (6). \( I_{N,S} \) and \( I_{N,T} \) are factors dependent on electron numbers to be calculated below.

We denote \( I_i = \langle L_i | R_i \rangle = \langle R_i | L_i \rangle \), where \( 1 \leq i < N \). \( L_i \) and \( R_i \) are wave functions (without spin part) based on Fock–Darwin states.

For \( N > 1 \), by applying the Slater–Condon rules \(^{15,20} \) we have

\[ I_{N,S} = I_{N}^2 = \sum_{j=1}^{N-1} I_{j}^2 \]

and

\[ I_{N,T} = I_{N}^2 = \sum_{j=1}^{N-1} I_{j}^2 \]

For unbiased case, we can express \( A_\Phi \) as

\[ A_\Phi = \frac{1}{2} \left[ \langle T(1, 2N - 1) | \rho(q) | T(1, 2N - 1) \rangle - \langle S(1, 2N - 1) | \rho(q) | S(1, 2N - 1) \rangle \right] \]

where \( A_\Phi(q) \) is obtained from the \( x \) and \( y \) components of orbital states.

\[ f(q_0) = \sin(q_0 a) \frac{-a^2}{(q_0 a)^2 - a^2} \]

where \( q_0 \) is a component of the momentum, \( a = 3 \times 10^{-9} \) m is width of the infinite square well for acoustic phonons. \(^{50} \)

For \( N = 1 \), the expression of \( A_\Phi \) has been explicitly shown in ref. [50]. Here, we give a general expression of \( A_\Phi \) for \( N > 1 \)

\[ \langle S(1, 2N - 1) | \rho(q) | S(1, 2N - 1) \rangle = \frac{e_q}{1 + I_{N,S}} \]

\[ \langle T(1, 2N - 1) | \rho(q) | T(1, 2N - 1) \rangle = \frac{e_q}{1 - I_{N,T}} \]

where

\[ e_q = \rho_{\uparrow, \downarrow} + \rho_{\downarrow, \uparrow} - 2 \sum_{j=1}^{N-1} \rho_{\uparrow, \downarrow} \rho_{\downarrow, \uparrow} \]

\[ + \sum_{j=1}^{N-1} \sum_{l=1}^{N-1} (I_{j} \rho_{\uparrow, \downarrow} \rho_{\downarrow, \uparrow} - 2 I_{l} \rho_{\uparrow, \downarrow}) \]

Here, \( I_1 = \langle L_1 | R_1 \rangle = \langle R_1 | L_1 \rangle \), and similarly, \( \rho_{\uparrow, \downarrow} = \langle L_1 | \rho | R_1 \rangle \).

We then have

\[ A_\Phi = \frac{2 \sin(I_1 \rho_{\uparrow, \downarrow} + I_2 \rho_{\downarrow, \uparrow})}{1 - I_1^2 - 2 I_2^2 \sum_{l=1}^{N-1} I_{l}^2} \]

\[ I_1 = -I_{\downarrow, \uparrow} + \rho_{\uparrow, \downarrow} + \rho_{\downarrow, \uparrow} \]

and

\[ I_2 = I_{\downarrow, \uparrow} + \rho_{\uparrow, \downarrow} + \rho_{\downarrow, \uparrow} \]

Here, it is straightforward to show that, for \( i < j \), we have \( I_i \ll 1, I_i \ll I_j \rho_{\uparrow, \downarrow} < \rho_{\uparrow, \downarrow}, \rho_{\downarrow, \uparrow} \ll \rho_{\downarrow, \uparrow} \).

For (1,1), (1,3), and (1,7), we have \( N = 1, 2, 4, \) therefore

\[ I_1 = 2 \sin(2 \sqrt{I_{\downarrow, \uparrow}^2 + I_{\uparrow, \downarrow}^2}) I_{\downarrow, \uparrow}^2 \]

\[ I_2 = 4 \sin^2(2 \sqrt{I_{\downarrow, \uparrow}^2 + I_{\uparrow, \downarrow}^2}) I_{\downarrow, \uparrow}^2 \]

\[ I_4 = 4 \sqrt{2} e^{-2 \sqrt{I_{\downarrow, \uparrow}^2 + I_{\uparrow, \downarrow}^2}} I_{\downarrow, \uparrow}^2 \]

Figure A2. Diagonal elements of DQD Hamiltonian occupied by eight electrons as function of detuning, in bases \{ | S(1, 2N - 1) \rangle, | T(1, 2N - 1) \rangle, | S(1, 2N - 1) \rangle, | T(1, 2N - 1) \rangle, | S(1, 2N - 1) \rangle, | T(1, 2N - 1) \rangle, | S(1, 2N - 1) \rangle, | T(1, 2N - 1) \rangle \}.
where \( l_l \) is left dot confinement length and \( l_r \) is right dot confinement length that can be calculated from their confinement strength. Therefore in Equation (B12) numerator, \( l_l^2 l_r^2 \ll l_l l_r \). As \( N \) increases, \( l_l \) and \( l_r \) also increases, eventually lead to increases of \( |A_A|^2 \) and the dephasing rate. One can also find that due to \( A_B \approx i l_r \), therefore \( |A_A|^2 \) decreases as \( x_q \) and \( h \omega_{hy} \) increase.

In biased case, the explicit expression of \( A_B \) at \( N = 1 \) can also be found in ref. [50]. For \( N > 1 \), there are two situations of biased case in our consideration. From Equation (9), we have

\[
A_B = \frac{1}{2}[(T(1, 2N - 1)|\rho(q)|T(1, 2N - 1)) - \langle S(0, 2N)|\rho(q)|S(0, 2N)\rangle]
\]

\[
= \frac{1}{2}[(T(1, 2N - 1)|\rho(q)|T(1, 2N - 1)) - \langle (S(1, 2N - 1)|\rho(q)|S(1, 2N - 1) = \langle 0|\rho(q)|0\rangle]
+ 2\beta\langle S(1, 2N - 1)|\rho(q)|S(0, 2N)\rangle
+ \beta^2\langle S(0, 2N)|\rho(q)|S(0, 2N)\rangle\langle 1 + \beta^2\rangle\]

and from Equation (10), we have

\[
A_B = \frac{1}{2}[(T(1, 2N - 1)|\rho(q)|T(1, 2N - 1)) - \langle S(2, 2N - 2)|\rho(q)|S(2, 2N - 2)\rangle]
\]

\[
= \frac{1}{2}[(T(1, 2N - 1)|\rho(q)|T(1, 2N - 1)) - \langle (S(1, 2N - 1)|\rho(q)|S(1, 2N - 1) = \langle 0|\rho(q)|0\rangle\]
+ 2\beta\langle S(1, 2N - 1)|\rho(q)|S(2, 2N - 2)\rangle
+ \beta^2\langle S(2, 2N - 2)|\rho(q)|S(2, 2N - 2)\rangle\langle 1 + \beta^2\rangle\]

where

\[
\langle S(0, 2N)|\rho(q)|S(0, 2N)\rangle = 2\sum_{i=1}^{N} \rho_{R_i,R_i}
\]

\[
\langle S(0, 2N)|\rho(q)|S(2, 2N - 2)\rangle = \frac{1}{\sqrt{2(1 + x_q N_N)}} \left( 4N \sum_{i=1}^{N-1} \rho_{R_i,R_i} - 2\sum_{i=1}^{N-1} \rho_{L_i,R_i} + 2\sum_{i=1}^{N-1} \rho_{R_i,L_i} \right)
\]

Appendix C: Merit Figures of Other Quantum Dot Parameters

In Figure C1, we show the merit figures calculated for three sets of parameters. Figure C1a shows a case with a short half dot distance \( x_q = 50 \) nm with a relatively strong confinement strength in the right dot \( h \omega_{hy} = 1.419 \) meV, while Figure C1b shows a case with an intermediate half dot distance \( x_q = 70 \) nm with a relatively weak \( h \omega_{hy} = 0.946 \) meV. In these cases, the barrier between the two dots is low, rendering the case with (1,7) electron occupancy ill-defined. Therefore only results for (1,3) and (1,1) are shown. We can see that the merit figure associated with (1,3) is clearly higher than those with (1,1), consistent with the findings in the

\[
\text{\textbf{Figure C1.} The merit figures versus the exchange interaction calculated for three different sets of parameters. a) } x_q = 50 \text{ nm, } h \omega_{hy} = 2.838 \text{ meV, } h \omega_{hy} = 1.419 \text{ meV. b) } x_q = 70 \text{ nm, } h \omega_{hy} = 2.838 \text{ meV, } h \omega_{hy} = 0.946 \text{ meV. c) } x_q = 80 \text{ nm, } h \omega_{hy} = 2.838 \text{ meV, } h \omega_{hy} = 1.419 \text{ meV.}}
\]

where, \( O(l_m^m \rho_{R_i,R_i}) \), \( m > 2 \) are higher-order terms that can be ignored due to the fact \( l_i \ll 1 \).
main text. In Figure C1c, results for all three cases of (1,7), (1,3), and (1,1) are shown. Again, these results are consistent with the main finding that in certain $j$ range, the merit figure for (1,7) is the highest, that for (1,3) is intermediate, and that for (1,1) is the lowest.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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