Coulomb interaction and valley-orbit coupling in Si quantum dots

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The valley-orbit coupling in a few-electron Si quantum dot is expected to be a function of its occupation number $N$. We study the spectrum of multivalley Si quantum dots for $2 \leq N \leq 4$, showing that, counterintuitively, electron-electron interaction effects on the valley-orbit coupling are negligible. For $N = 2$ they are suppressed by valley interference, for $N = 3$ they vanish due to spinor overlaps, and for $N = 4$ they cancel between different pairs of electrons. To corroborate our theoretical findings, we examine the experimental energy spectrum of a few-electron metal-oxide-semiconductor quantum dot. The measured spin-valley state filling sequence in a magnetic field reveals that the valley-orbit coupling is definitively unaffected by the occupation number.

I. INTRODUCTION

The requirements of quantum bit (qubit) scalability and long coherence times have brought solid-state spin systems to the fore of quantum computation.1−3 Realizing spin qubits in Si quantum dots is particularly promising thanks to the remarkable coherence properties of Si4,5 and significant experimental progress has lately been reported.6−11 The valley degree of freedom of Si12−15 is vital in quantum computing,16−20 it enables valley-based information processing21−23 and resonance24 but hampers spin qubit.25 A valley-orbit coupling (VOC) causes valley states to hybridize into valley eigenstates26−28 and the biggest issues at present are an understanding of the magnitude of the VOC, its response to applied fields, and its sensitivity to interactions with the environment and among electrons.

The VOC of singly occupied quantum dots stems from the interface potential,29 yet for few-electron quantum dots, interactions contribute to the VOC. Since Coulomb repulsion depends on the spatial separation of electrons, it is often appreciable in quantum dots, where electrons are strongly confined. The on-site interaction $u$ can exceed the confinement energy, and in Si double quantum dots repulsion contributes sizably to interdot tunneling.30 The relative contribution of interactions to the VOC of few-electron quantum dots is an issue of substantial conceptual and practical significance.

This paper is a theoretical and experimental study of interaction effects on the VOC in a single Si quantum dot with $1 \leq N \leq 4$. For $N = 2$, we show that the Coulomb interaction effect on the VOC is suppressed by valley interference, while for $N = 3$ and $N = 4$ interaction terms vanish due to spinor overlaps. Experimental data supports this finding, showing no evidence of interactions in the valley-orbital spectrum of Si quantum dots with $1 \leq N \leq 3$. We argue that these observations apply beyond $N = 4$.

The outline of this paper is as follows. In Sec. [I] we introduce the model of the quantum dot, and discuss the spectrum for $1 \leq N \leq 4$. In Sec. [II] we compare our theoretical findings with experimental data. Sec. [IV] is devoted to a discussion of the underlying physics, and is followed by a summary and conclusions.

II. MODEL

We consider a dot located at the origin with Fock-Darwin radius $a$. The confinement potential

$$V_D(x, y, z) = \frac{\hbar}{2m^*a^2} (x^2 + y^2) + U_0\theta(-z) + eFz,$$

(1)

with the electron charge $-e$, in-plane effective mass $m^*$, interface potential $V_z = U_0\theta(-z)$, $\theta$ the Heaviside function, and gate electric field $F$.

The electron wave functions $D_\xi(x, y, z) = \phi_D(x, y, z)\psi(z)u_\xi(r)e^{ikz}$, the valley index $\xi = \{\pm, -z\}$, and $k_{z=\pm z} = \pm k_0 = \pm 0.85(2\pi/a_{Si})$, with $a_{Si} = 5.43\text{Å}$ the Si lattice constant. The envelope $\phi_D(x, y) = \frac{1}{a\sqrt{\pi}}e^{-(x^2+y^2)/a^2}$, while $\psi(z) = N_{\xi=\pm}e^{k_0z/2}\theta(z) + N(z = z_0)e^{-k_{z=\pm z}/2}\theta(z)$ is a variational envelope function, with $k_{Si}$ a variational parameter, $k_0$ fixed, and $N$ the normalization.22 Given the twofold spin and valley degrees of freedom, the lowest single-particle levels can accommodate up to 4 electrons [see Fig. [I] (a)]. For $N \leq 4$ the number of many-electron states is the combination $C_N^1$. The case $N = 1$ has been studied at length, and the bare (single-particle) VOC is $\Delta_0 \equiv |\Delta_0|e^{-i\phi_0} = (D_z|U_0\theta(-z) + eFz|D_{-z})$. The valley-orbit splitting is $2|\Delta_0|$, and the valley eigenstates are $D_\pm = (1/\sqrt{2})(D_z \pm e^{i\phi_0}D_{-z})$.22

A. Two-electron case

For $N = 2$ the Hamiltonian $H_{ee} = T^{(1)} + V_D^{(1)} + T^{(2)} + V_D^{(2)} + V_{ee}$ where superscripts $i \in \{1, 2\}$ label electrons at $r_1$ and $r_2$, $T$ is the kinetic energy, and $V_{ee} = \frac{e^2}{4\pi\epsilon_0\epsilon_r|r_1-r_2|}$
is the Coulomb interaction, with \( \varepsilon_0 \) the permittivity and \( \varepsilon_r \) the relative permittivity. The \( C_2^2 = 6 \) two-particle states are 3 spin singlets (\( \phi^S \)) and 3 spin triplets (\( \phi^T \)),

\[
\phi^S_{\pm \pm \pm \pm} = D^{(1)}_{\pm \pm} D^{(2)}_{\pm \pm} \chi_S
\]

\[
\phi^S_{\text{mix}} = \frac{1}{\sqrt{2}} (D^{(1)}_{\pm} D^{(2)}_{-} \pm D^{(1)}_{-} D^{(2)}_{\pm}) \chi_S T,
\]

with \( \chi_S \) and \( \chi_T \) spin the singlet and triplet spin wave functions, given by

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

\[
|\chi_{T,\uparrow\uparrow}\rangle = |\uparrow\downarrow\rangle
\]

\[
|\chi_{T,\downarrow\downarrow}\rangle = |\downarrow\uparrow\rangle
\]

\[
|\chi_{T,0}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)
\]

We use \(|\chi_T\rangle\) generically for any of the three triplet wave functions.

In the basis \( \{\phi^S_{\pm \pm \pm \pm}, \phi^S_{\text{mix}}, \phi^T\} \), the two-electron Hamiltonian can be written as

\[
H_{\text{val}} = 2(\varepsilon_0 + u)I + H_{\text{val}}, \quad \varepsilon_0 = \langle D^{(1)}_{\xi_1} | [T^{(i)} + V_D] D^{(2)}_{\xi_1} \rangle, \quad u = \langle D^{(i)}_{\xi_1} D^{(2)}_{\xi_2} | V_{\text{ee}} | D^{(2)}_{\xi_1} D^{(i)}_{\xi_1} \rangle,
\]

with \( \Delta_{\text{ee}} = \langle D^{(1)}_{z} D^{(2)}_{-z} | V_{\text{ee}} | D^{(2)}_{z} D^{(1)}_{-z} \rangle \). The eigenvalues of \( H_{\text{val}} \) are 0, \( -\Delta_{\text{ee}} \) and \( \Delta_{\pm} = \pm \sqrt{\Delta_{ee}^2 + 16(\Delta_0)^2} \), plotted in Fig. 2 as functions of \( \Delta_{ee} \). We note the crossover of eigenvalues in Fig. 2. At large \( \Delta_0 \gg \Delta_{ee} \), the ground state is a spin singlet, yet when \( \Delta_0 \) is small enough, the ground state corresponds to the eigenvalue \( -\Delta_{ee} \), and is a spin triplet. In such a case the ground state will move down in energy in a non-zero magnetic field.

To assess the possibility of a triplet ground state, we evaluate \( \Delta_{ee} \). We expand \( u_z(r) = \sum_K c_K e^{iK \cdot r} \), with \( K \) reciprocal lattice vectors, switch to center of mass and relative variables \( r = \mathbf{r}_1 - \mathbf{r}_2, \mathbf{R} = \mathbf{r}_1 + \mathbf{r}_2 \), and employ cylindrical polar coordinates. The integration over \( \mathbf{R} \) is trivial, while over \( r = (r_\perp, \phi, z) \) we make the substitution

\[
\frac{1}{r} = \frac{2}{\sqrt{\pi}} \int_0^\infty dt e^{-t^2} t^2,
\]

reducing the problem to

\[
\Delta_{ee} = \frac{e^2 \Sigma}{2 c_0 \varepsilon_0 \varepsilon_r \sqrt{\pi}} \int_0^\infty du \cos(2k_0 u) e^{z^2} \text{Erfc} \left( \frac{u}{a \sqrt{2}} \right) L(u),
\]

with

\[
\Sigma = \sum_{K_1 K_2 Q_1 Q_2} c^{+*}_{K_1} c^{+*}_{K_2} c^{*}_{K_1-Q_1} c^{*}_{K_2-Q_2}, \quad \text{Erfc} \text{ the complementary error function and}
\]
\[
L(u) = \frac{2\pi N a^4}{k_0} e^{-k_0 u} + \frac{2\sqrt{2}\pi N a^4}{\delta k_0} e^{-k_0 u} e^{\delta_k u} e^{\delta_k z_0 (u + z_0)^2 - 2 e^{\delta_k u} (u + z_0)^2} + \frac{N^4 \pi}{\sqrt{2 k_{z_0}^2}} e^{-k_{z_0} u} [2 k_{z_0}^2 (u + z_0)^2 + 2 k_{z_0}^2 (u + z_0) (u + 2 z_0) + k_{z_0}^2 (u^2 + 6 u z_0 + 6 z_0^2) + 3 k_{z_0} (u + 2 z_0) + 3]
\]

(6)

Using \( a = 10 \text{nm} \) as the lowest realistic quantum dot radius, the effective \( c_e = 7.9 \) for a sample Si/SiO\(_2\) interface, the parameters of Ref. [22] for the variational wave function and the coefficients \( c_k \) of Ref. [27] we obtain numerically \( \Delta_{ee} = 0.0352 \text{meV} \). The Coulomb interaction contribution to the VCO is negligible compared to the single-particle term \( \Delta_0 \), which is of the order of 0.05 meV [22].

B. Three-electron case

We consider next \( N = 3 \). The quantum dot can be in one of \( C^3_v = 4 \) states. Using \( | \uparrow \rangle, | \downarrow \rangle \) for up and down spinors respectively, one sample wave function is the Slater determinant

\[
\phi_1^{3e}(z \uparrow, \neg z \uparrow, z \downarrow) = \frac{1}{\sqrt{6}} \begin{vmatrix} D_{z \uparrow}^{(1)} & D_{z \uparrow}^{(2)} & D_{z \uparrow}^{(3)} \\
D_{z \uparrow}^{(2)} & D_{z \uparrow}^{(3)} & D_{z \uparrow}^{(1)} \\
D_{z \uparrow}^{(3)} & D_{z \uparrow}^{(1)} & D_{z \uparrow}^{(2)} \end{vmatrix},
\]

(7)

and analogously \( \phi_2^{3e}(z \uparrow, \neg z \downarrow, z \downarrow), \phi_3^{3e}(z \downarrow, \neg z \uparrow, \neg z \downarrow), \) and \( \phi_4^{3e}(z \downarrow, \neg z \uparrow, \neg z \downarrow) \). The 3-electron Hamiltonian

\[ H_{3e} = \sum_{i=1}^{3} \hat{T}^{(i)} + V_D + \frac{1}{2} \sum_{i \neq j} V_{ee}. \]

Each basis state contains 6 terms, and each Hamiltonian matrix element has 36 terms. Spinor overlaps annihilate most of them, since the Coulomb interaction is spin-independent. We calculate \( \langle \phi_1^{3e} | H_{3e} | \phi_1^{3e} \rangle \) as an example. The six terms in \( \phi_1^{3e} \) are \( \phi_{11} = D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \uparrow}^{(3)} \),

\[
\phi_{12} = -D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \downarrow}^{(3)}, \quad \phi_{13} = D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \downarrow}^{(3)} + D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \downarrow}^{(3)}, \quad \phi_{14} = -D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \downarrow}^{(3)}, \quad \phi_{15} = D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \downarrow}^{(3)}, \quad \phi_{16} = -D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \downarrow}^{(3)}. \]

We obtain

\[
\langle \phi_{11} | H_{3e} | \phi_{11} \rangle = \sum_{i=1}^{3} \langle D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \uparrow}^{(3)} | (z \uparrow) | D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \uparrow}^{(3)} \rangle + \langle (3) | D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \uparrow}^{(3)} | (1) \rangle D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \uparrow}^{(3)} \rangle = 3 \Delta_0 + 3 \Delta_0.
\]

\[
\langle \phi_{11} | H_{3e} | \phi_{12} \rangle = -\langle (1) | D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \uparrow}^{(3)} | H_{3e} | (1) \rangle D_{z \uparrow}^{(1)} D_{z \uparrow}^{(2)} D_{z \uparrow}^{(3)} \rangle = -\Delta_{ee},
\]

(8)

and \( \langle \phi_{11} | H_{3e} | \phi_{12} \rangle = \langle \phi_{11} | H_{3e} | \phi_{12} \rangle + \langle \phi_{11} | H_{3e} | \phi_{13} \rangle = \langle \phi_{11} | H_{3e} | \phi_{14} \rangle = 0 \). Adding up these terms gives \( \langle \phi_1^{3e} | H_{3e} | \phi_1^{3e} \rangle = 3 \Delta_0 + 3 \Delta_0 \), and similarly \( \langle \phi_1^{3e} | H_{3e} | \phi_1^{3e} \rangle = -\Delta_0 \). The matrix elements \( \langle \phi_1^{3e} | H_{3e} | \phi_2^{3e} \rangle \) and \( \langle \phi_1^{3e} | H_{3e} | \phi_3^{3e} \rangle \) vanish because no terms in the bra and ket states share the same spin arrangement. Analogous arguments apply to all the remaining matrix elements, yielding

\[
H_{3e} = (3 \Delta_0 + 3 \Delta_0) \mathbb{1} + \begin{pmatrix} 0 & 0 & 0 & -\Delta_0 \\
0 & 0 & \Delta_0 & 0 \\
0 & \Delta_0 & 0 & 0 \\
-\Delta_0 & 0 & 0 & 0 \end{pmatrix}
\]

(9)

The finite matrix elements of \( H_{3e} \) are \( \langle \phi_1^{3e} | H_{3e} | \phi_1^{3e} \rangle = 3 \Delta_0 + 3 \Delta_0 \) (for \( 1 < n < 4 \) and \( \langle \phi_1^{3e} | H_{3e} | \phi_3^{3e} \rangle = -\Delta_0 \)). The eigenvalues are \( 3 \Delta_0 + 3 \Delta_0 - \Delta_0 = \Delta_0 \). As a result of spinor overlaps, the Coulomb term \( \Delta_{ee} \) does not appear in the off-diagonal matrix elements and does not contribute to the valley splitting, giving only an identical offset to all the energy eigenvalues.

C. Four-electron case

For \( N = 4 \), all four lowest-energy single-particle states are occupied, and only \( C^4_v = 1 \) many-particle state exists. The Slater determinant wave function \( \phi_{4e} \) for \( N = 4 \) takes the form

\[
\phi_{4e} = \frac{1}{\sqrt{24}} \begin{vmatrix} D_{z \uparrow}^{(1)} & D_{z \uparrow}^{(1)} & D_{z \uparrow}^{(1)} & D_{z \uparrow}^{(1)} \\
D_{z \uparrow}^{(2)} & D_{z \uparrow}^{(2)} & D_{z \uparrow}^{(2)} & D_{z \uparrow}^{(2)} \\
D_{z \uparrow}^{(3)} & D_{z \uparrow}^{(3)} & D_{z \uparrow}^{(3)} & D_{z \uparrow}^{(3)} \\
D_{z \uparrow}^{(4)} & D_{z \uparrow}^{(4)} & D_{z \uparrow}^{(4)} & D_{z \uparrow}^{(4)} \end{vmatrix}.
\]

(10)
as either a quantum dot or a 2DEG reservoir, depend-
ing on the extent of planar confinement provided by the
gates. The details of the fabrication process and
typical bias configurations are reported elsewhere. A
schematic diagram of the device used is shown in Fig. 1(b).
The system works as a single-lead quantum dot
capacitively coupled to a single-electron-transistor (SET)
acting as a charge sensor. Independent gate electrodes
control the occupancy of the quantum dot, the tunnelling
rate between the dot and the reservoir, the Fermi energy
of the reservoir, and the bias point of the SET detector.
The dot is reliably operated in the few-electron regime
down to the last electron.

The excitation spectrum of the quantum dot is mea-
sured using a pulsed voltage technique. A train of
square voltage pulses at a frequency of few hundreds Hz
is applied to the gate that directly affects the quantum
dot potential (in addition to its DC voltage). This shifts
the energy levels of the dot in time, inducing charge tran-
sitions whenever the dot’s single-particle levels come into
resonance with the lead’s Fermi energy. An electron can
be loaded from the reservoir into the dot during the upper
phase of the pulse and unloaded during the lower phase
(as shown in Fig. 3(a)). The time-dependent gate volt-
age modulates the sensor current, $I_{SET}$, via capacitive
effects, and a lock-in amplifier selects the spectral com-
ponent which is uniquely associated to tunneling events
(i.e. the one at the frequency of the pulse). This tech-
nique allows one to probe both ground and excited states
for each $N$, as long as the relaxation rate is slower than
the pulse frequency and the pulse magnitude spans the
relevant energy separation. The measured spectrum re-
vals that the energy separation between the first excited
orbital state and the ground state varies between 1-8meV
according to dot’s occupancy. A comprehensive descrip-
tion of the measurement set-up and parameters is found
in Ref. 39.

In Fig. 3(b) measurements of the spin-valley states’
evolution in a magnetic field $B \parallel [110]$ (parallel to the
Si/SiO$_2$ interface) are shown for $1 \leq N \leq 3$. Each data
point indicates a maximum in the differential sensing cur-
tent signal for varying DC gate voltage bias and a fixed
pulse amplitude of 20 mV. The energy scale on the y-axis
is obtained by converting the gate voltage into electro-
chemical potential using the appropriate lever arm con-
version factor ($\approx 0.3$ eV/V). The vertical shift of each
trace is arbitrary and does not reflect the quantum dot
charging energy. A strong sensing signal is due to charge
transfers to/from the quantum dot. Hence, the observed
magnetic field dependence maps the filling of spin-valley
states for individual electrons. The slope of $E(B)$ is given
by $\frac{\partial E}{\partial B} = -g\mu_B B \Delta S_{\text{tot}}(N)$, where $g$ is the electron gy-
romagnetic ratio, $\mu_B$ is the Bohr magneton and $\Delta S_{\text{tot}}(N)$
is the change in total spin when the $N$-th electron is
added to the dot. Hence, a slope of $g\mu_B$ indicates a
spin-up addition, while a slope of $-g\mu_B$ is due to a spin-
down electron. Solid lines shown in Fig. 3(b) are guides
for the eye with slopes $\pm g\mu_B$. Using $g = 2$ for bulk Si.

To understand the interplay between spin and valley

III. EXPERIMENTAL SPIN-VALLEY SPECTRUM

To experimentally probe the effect of Coulomb interac-
tions on the VQC, we use quantum dots fabricated with
metal-oxide-semiconductor (MOS) technology in nearly
intrinsic Si. In these devices a three-layer Al-Al$_2$O$_3$-
Al gate stack allows one to electrostatically modulate
the conduction band profile near the Si/SiO$_2$ interface.
As a result, an electron accumulation layer is selectively
formed in the semiconductor substrate and can function
as either a quantum dot or a 2DEG reservoir, depend-

![Figure 3: (a) Energy diagrams of the dot when voltage pulses are superimposed to the DC bias. When a single-particle level is near the reservoir’s Fermi level, an electron can be loaded into the dot during the upper phase of the pulse (solid lines) and unloaded during the lower phase (dashed lines). (b) Magnetic field dependence of the spin-valley states filling for $N \leq 3$, where $D\pm$ label single-electron valley eigenstates and $S$, $T\pm$ label spin states, consistent with Eq. 3. Data points show where the differential sensor’s signal $\delta E/\delta B$ is maximized. Solid lines are guides for the eye with slopes $\pm g\mu_B/2$ in red and $-g\mu_B/2$ in green. Boxes of different colors indicate different valley occupancies. Blue (black) arrows represent the spin state of the current (previous) electron addition(s). Sets of data for different charge transitions are arbitrarily shifted in energy for clarity. (c) Energy diagram of the 1-electron spin-valley states evolution in magnetic field. At the field value $B = B_0$ the two valley states cross, and Zeeman and valley-orbit splittings coincide. Dashed lines indicate states that are not probed in the experiments.]

The energy $\langle \phi_{\text{el}} | H_4 | \phi_{\text{el}} \rangle = 4\varepsilon_0 + 6u$ contains no inter-
valley terms, stemming from either the bare VOC or the
Coulomb interaction, since interaction terms cancel be-
tween pairs of electrons with different spinors.
degrees of freedom in a magnetic field, we analyse individual charge additions. The first transition ($N = 0 \rightarrow 1$) reveals that for low magnetic fields the slope is positive up to $B = B_k \approx 2T$, where a change of sign occurs; hence, a spin-up (spin-down) electron is loaded into the dot for low (high) B-fields. For the first electron addition, one would expect to fill the spin-down lower valley eigenstate (the ground state) at all B-field values (see red dashed line in Fig. 3(c)). However, the measurements indicate that the excited (ground) state of the lower $D_-$ (upper $D_+$) valley is probed for this transition for $B < B_k$ ($B > B_k$). This occurs because the tunnelling rate between the dot and the lead in our measurement is faster than the relaxation rate, so that the largest contribution to the sensing signal comes from the loading/unloading of the excited states. Using Fig. 3(c) we can explain the presence of the kink (change of slope sign). For increasing magnetic fields the states $|D_-\rangle$ and $|D_+\rangle$ cross, making it energetically favourable for a spin-down electron to charge the dot. The position of the kink reveals the valley-orbit splitting, which coincides with the Zeeman splitting, as $g\mu_B B_k = 0.23$ meV, yielding $|\Delta_0| = 0.115$ meV.

The trend in Fig. 3(b) for the $N = 1 \rightarrow 2$ transition is similar to that for $N = 0 \rightarrow 1$. The ground state for $N = 1$ is spin-down for all B. The spin-filling measurements reveal that for low B a spin-up electron is added to form a singlet which fully occupies the $-$ valley eigenstate. However, at larger B, a kink occurs at the same $B_k$ as for $N = 1$. This suggests that for $B > B_k$ a spin-down electron is added to form the triplet $|\phi_{mix}\rangle$. The antisymmetry of the 2-electron wave-function requires one electron to occupy an excited state; here, this is the $+$ valley eigenstate, which is significantly lower than the first excited orbital state. The observed change of slope is due to a singlet-triplet crossing and, once again, the Zeeman and valley-orbit splittings coincide at $B = B_k$.

For $N = 2 \rightarrow 3$, we again observe a change of slope at $B = B_k$, but unlike the previous cases, the electron added at low (high) fields is spin-down (spin-up). To understand this, we note that for $B < B_k$ the 2-electron ground state is a spin singlet that fully occupies the lower valley eigenstate. The next available state would be a spin-down in the upper valley eigenstate. However, for $B > B_k$ the 2-electron ground state switches to $|\phi_{mix}\rangle$, which would allow one more electron in the lower electron valley eigenstate. This can only be spin-up because of Pauli exclusion. The change of slope at the same field value as for the previous transitions confirms that $|\Delta_0| = 0.115$ meV for $N = 3$ as well. These measurements confirm that the VOC is independent of $N$ up to $N = 3$, corroborating the prediction that $\Delta_{ee}$ is negligible.

V. SUMMARY

In conclusion, we have demonstrated theoretically and experimentally that in few-electron quantum dots the VOC has no significant contribution from electron-electron interactions. We expect these findings to be generalizable to $N > 4$, since valley interference and spinor overlaps are equally relevant to higher orbital excited states. Conceptually, this proves that interactions are not sharp enough in real space to couple valleys, which have a large separation in $k$-space. Together with previous research, it shows that the VOC is fully determined by the properties of the interface: the size and shape of the interface potential step, electric field and roughness profile.

These findings will aid experimentalists working on quantum computing in Si and other materials with valleys, such as C and Ge. The valley degree of freedom can be a significant impediment to single-spin and singlet-triplet qubits, and it is essential for their operation that the VOC be fully characterised, since valleys complicate the spin state spectrum on a fundamental level. The size of the VOC and its sensitivity to interactions and occupation number is also a critical ingredient of valley qubit, which may reduce sensitivity to noise.
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