Hybrid Spin and Valley Quantum Computing with Singlet-Triplet Qubits

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The valley degree of freedom in the electronic band structure of silicon, graphene, and other materials is often considered to be an obstacle for quantum computing (QC) based on electron spins in quantum dots. Here we show that control over the valley state opens new possibilities for quantum information processing. Combining qubits encoded in the singlet-triplet subspace of spin and valley states allows for universal QC using a universal two-qubit gate directly provided by the exchange interaction. We show how spin and valley qubits can be separated in order to allow for single-qubit rotations.

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An alternative to single-spin qubits in quantum dots [1] is to encode each qubit in a double quantum dot (DQD) within the two-dimensional subspace spanned by the spin singlet $|S\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$ and the triplet $|T_0\rangle = (|01\rangle + |10\rangle)/\sqrt{2}$ [2], with $|0\rangle = |\uparrow\rangle$, $|1\rangle = |\downarrow\rangle$. For this singlet-triplet qubit, single-qubit rotations can be realized by the exchange interaction [3,4] and a gradient in the magnetic field [4]; two-qubit gates have been proposed based on exchange interaction [5–8] or electrostatic coupling [9–11]. An electrostatically controlled entangling gate has been realized experimentally [12,13]. Quantum computing (QC) with single-spin and/or single-valley qubits requires rotations of single-valley and/or single-spin degrees of freedom (DOFs) [14]. In this Letter, we show that, by extending the concept of S-T_0 qubits to electrons with spin and valley DOFs, the exchange interaction together with Zeeman gradients directly provides universal QC. Single-qubit rotations are feasible when the spin and the valley S-T_0 qubits are stored in separated DQDs, whereas in a dual-used DQD, i.e., containing the S-T_0 spin and valley qubits, a two-qubit gate is obtained by exchange interaction [14]. Here, we focus on operations separating and bringing together spin and valley qubits, allowing for a universal set of single- and two-qubit operations in a quantum register.

The valley DOF describes the existence of nonequivalent minima (maxima) in the conduction (valence) band in several materials such as silicon [15], graphene [16], carbon nanotubes [17], aluminum arsenide [18], or transition metal dichalcogenide monolayers [19,20]. A twofold valley degeneracy can be considered as a qubit. In particular, silicon-based heterostructures have aroused much interest as hosts for electron spin qubits [15] due to long relaxation [21] and coherence [22] times. Valley states in silicon structures have been under intense theoretical [23–38] and experimental [39–52] investigation recently. The valley degeneracy is often considered problematic for spin QC [53,54], and valley splitting is used to achieve pure spin exchange interaction [55]. Also, theories for the manipulation of valley qubits have been developed for carbon nanotubes [56], graphene [57,58], and silicon [59–61]. While these approaches consider valley and spin qubits separately, we investigate a hybrid quantum register containing both spin and valley qubits.

Two different types of hybrid spin-valley singlet-triplet quantum registers will be studied (Fig. 1). Both setups comprise two kinds of DQDs: one (e.g., dots I and III) with a spin DOF only (simple yellow circles), where the valley

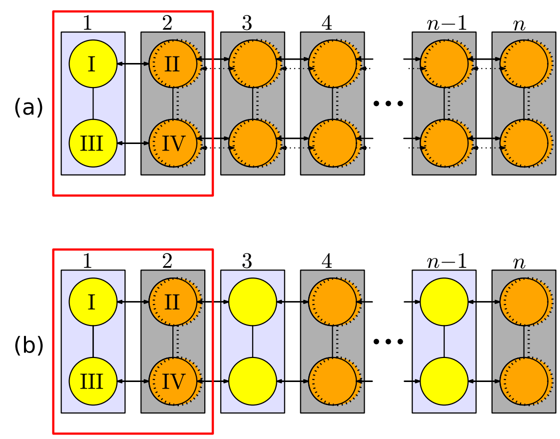

FIG. 1 (color online). Two quantum registers for QC with spin and valley singlet-triplet qubits. The single (yellow) circles denote dots with spin DOF only (valley degeneracy lifted) hosting auxiliary spins, whereas the double (orange) circles denote dots with both spin and valley DOFs storing one spin and one valley S-T_0 qubit. The lines within the DQDs represent the exchange interaction (a single line for spin-only dots, solid and dotted lines for spin and valley), which can realize single-qubit gates when the spin qubit is transferred to the spin-only DQD and a two-qubit gate when spin and valley qubits are in the same DQD. The arrows between dots from neighboring DQDs represent SWAP operations, interchanging the spin (solid arrow) or valley (dotted arrow) state between these dots. Register (b) has more auxiliary dots; quantum gate sequences are shorter than in (a).

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degeneracy does not exist or has been lifted and another kind of DQD (e.g., II and IV) with both spin and twofold valley DOF (double orange circles). The elementary building block of the proposed quantum register consists of two DQDs, one of each kind (red rectangle in Fig. 1). We use the singlet $|S\rangle$ and triplet $|T_0\rangle$ states of spin and valley in DQD 2 as the logical qubits. The spins in DQD 1 are spin polarized, $|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$, which is needed for the single-qubit gates. The exchange interaction between dots II and IV, described in general by a Kugel-Khomskii Hamiltonian [14,62], already leads to a universal two-qubit gate between the spin and the valley singlet-triplet qubits in the same DQD [14]. Single-qubit gates for the logical qubits can be achieved by applying two spin-only SWAP gates, between I and II and between III and IV, interchanging the spin S-T_0 qubit in DQD 2 with the polarized ancilla spins in DQD 1, without affecting the valley state. The single-qubit gates of the spin and the valley qubits can be realized by exchange interaction and a spin or valley Zeeman gradient [4,60]. State preparation and measurements can be done for spatially separated spin and valley qubits. Changing the detuning within the DQD maps exactly one state of the qubit to a state with both electrons in one dot due to the Pauli exclusion principle [63,64]. The charge state can be detected by a quantum point contact [3]. State preparation works in the opposite direction, starting from a ground state with both electrons in one dot at large detuning. Before explaining how to perform arbitrary quantum gates in the registers, we propose a realization of an elementary gate in our scheme, the spin-only SWAP gate.

Model.—We consider the system consisting of dots I and II in Fig. 1, i.e., one dot with a spin DOF only and the other dot with spin and twofold valley DOF. We model the physics in this DQD by the Hamiltonian $H = H_0 + H_T + H_V$. The influence of the detuning ε and the Coulomb repulsion energy between two electrons on the same site, U, is given by $H_0 = \varepsilon(\hat{n}_1 - \hat{n}_2)/2 + U\sum_{i=1,2}\hat{n}_i(\hat{n}_i - 1)/2$ with the number operators $\hat{n}_1 = \sum_s \hat{c}^\dagger_{1s}\hat{c}_{1s}$ and $\hat{n}_2 = \sum_{s,v}\hat{c}^\dagger_{2sv}\hat{c}_{2sv}$, where $\hat{c}^{(\dagger)}_{1s}$ annihilates (creates) an electron with spin $s = \uparrow, \downarrow$ in dot I and $\hat{c}^{(\dagger)}_{2sv}$ annihilates (creates) an electron with spin $s = \uparrow, \downarrow$ and valley $v = \pm$ in dot II. Electron hopping is described by $H_T = \sum_{s,v} t_v \hat{c}^\dagger_{1s}\hat{c}_{2sv} + \mathrm{H.c.}$, and the valley splitting by $H_V = h\sum_s(\hat{c}^\dagger_{2s+}\hat{c}_{2s+} - \hat{c}^\dagger_{2s-}\hat{c}_{2s-}) \equiv h\sigma_z$, where σ_z is a Pauli matrix acting on the valley space. The sums run over $s = \uparrow, \downarrow$ and $v = \pm$. The valley-dependent hopping elements $t_\pm$ can be expressed by [59] $t_\pm = t(1 \pm e^{i\varphi})/2$ with real parameters t and φ, and h can be tuned in silicon by the electrically controlled confinement potential [45] and in graphene by an out-of-plane magnetic field [65]. For two electrons in dots I and II, there are 15 possible states: one with (2,0), six with (0,2), and eight with (1,1) charge distribution between dots I and II. In the limit $t \ll |h + (U \pm \varepsilon)|, |h - (U \pm \varepsilon)|$, a Schrieffer-Wolff transformation [66] yields the effective Hamiltonian (see the Supplemental Material [67])

$$H_{\mathrm{eff}} = [(A\cos\varphi + B)\mathbb{1} + (A + B\cos\varphi)\sigma_z + B\sin\varphi\sigma_y]P_S + \tilde{h}\sigma_z + C[(1-\cos\varphi)\mathbb{1} - \sin\varphi\sigma_y]. \tag{1}$$

Here, P_S is the projector on the spin singlet $|S\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, $A = 4t^2Uh\varepsilon/[(h-U-\varepsilon)(h+U-\varepsilon)\times(h-U+\varepsilon)(h+U+\varepsilon)]$, $B = A(h^2+\varepsilon^2-U^2)/2h\varepsilon$, $\tilde{h} = h\{1 + t^2(1-\cos\varphi)/[2(h-U+\varepsilon)(h+U-\varepsilon)]\}$, and $C = t^2(U-\varepsilon)/[2(h-U+\varepsilon)(h+U-\varepsilon)]$. Note that H and H_{eff} are block diagonal in the spin singlet-triplet basis, similar to the situation in Ref. [59]. We aim at using the term proportional to P_S to perform a spin-only SWAP gate, interchanging the spin information of dots I and II independently of the valley state. We will show that this is possible despite the valley dependence of H_{eff}.

Spin-only SWAP *gate.*—For the valley-degenerate case $h = 0$, Eq. (1) simplifies to the exchange Hamiltonian

$$H^0_{\mathrm{eff}} = -JP_SP_k - \tilde{J}P_{k^\perp}, \tag{2}$$

where $J = 4t^2U/(U^2 - \varepsilon^2)$ and $\tilde{J} = t^2/(U - \varepsilon)$. The first term is proportional to P_S and to the projector P_k on the valley state $|k\rangle = [(1 + e^{-i\varphi})|+\rangle + (1 - e^{-i\varphi})|-\rangle]/2$ occupied by an electron after hopping from dot I to dot II. The second term is spin independent and $\propto P_{k^\perp} = |k^\perp\rangle\langle k^\perp|$, where $|k^\perp\rangle = [(1-e^{-i\varphi})|+\rangle + (1+e^{-i\varphi})|-\rangle]/2$ is orthogonal to $|k\rangle$. Both contributions originate from the Pauli principle: virtual hopping between dots I and II is possible only if the participating (0,2) or (2,0) state is antisymmetric. Virtual hopping from (1,1) to (0,2) and back is $\propto t^2/(U - \varepsilon)$ and dominates for $\varepsilon \approx U$; if the valley state in the right dot is $|k^\perp\rangle$, this channel is open, independently of the spin states, as the valley state $|k\rangle$ used within the virtual hopping is empty. If the valley state is $|k\rangle$, the spins have to be in a singlet to allow for an antisymmetric (0,2) state. Virtual hopping from (1,1) to (2,0) and back requires a valley state $|k\rangle$ in the right dot, as $|k^\perp\rangle$ has no overlap with the state in the left dot; it further requires the spins to be a singlet to obey Fermi-Dirac statistics.

For $|U + \varepsilon| \ll U$, $\tilde{J}$ can be neglected and the time evolution $U_0(\phi) = \exp[-i\int_0^\tau d\tau' H^0_{\mathrm{eff}}(\tau')/\hbar]$ with $\phi = \int_0^\tau d\tau' J(\tau')/\hbar$ can be computed easily: $U_0(\phi) = \mathbb{1} + (e^{i\phi} - 1)P_SP_k$. If the conditions $\tilde{J} \approx 0$, $\varphi = \pi/2$, and controllability of the valley splitting h are fulfilled, we obtain a spin-only SWAP gate with the sequence $\mathrm{SWAP} \equiv \mathbb{1} - 2P_S = \sigma_z U_0(\pi)\sigma_z U_0(\pi)$. Here, h is turned off or at least made negligibly small during the exchange interaction but dominates over exchange in between to realize the valley gate σ_z.

If $\tilde{h}\sigma_z$ is the dominant contribution in H_{eff}, we find parameters which allow for a spin SWAP gate (Figs. 2

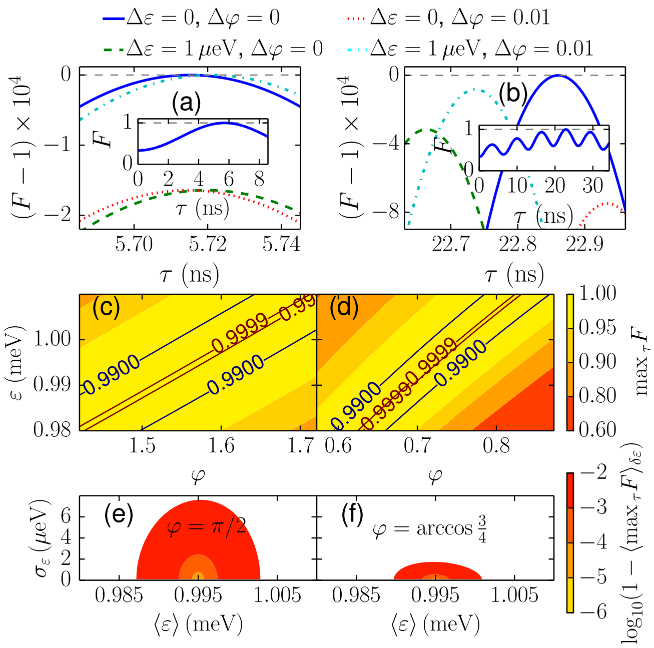

FIG. 2 (color online). Fidelity F of the time evolution operator $U_{\mathrm{eff}}(\tau)$ describing the exchange interaction between a spin-only dot and a spin-valley dot with respect to the spin SWAP gate according to Eq. (3). The parameters are chosen to be $U = 1$ meV, $h = 0.1$ meV, and $t = 6$ μeV. (a),(b) F maximized over the gate time τ (scale bar). The detuning is chosen to be $\varepsilon = \sqrt{U^2 - h^2} + \Delta\varepsilon \approx 0.995$ meV $+ \Delta\varepsilon$ and the phase in the hopping matrix elements, $\varphi = \pi/2 + \Delta\varphi$ (a) and $\varphi = \arccos\frac{3}{4} + \Delta\varphi$ (b). (c),(d) Contour plots of maximal fidelity in dependence of ε and φ. The maximum over τ is taken numerically by searching around the first (c) and fourth (d) local maximum. At $\Delta\varphi = 0$, $\Delta\varepsilon = 0$, $F = 1$ can be realized. A shift in the valley hopping phase, $\Delta\varphi$, can be compensated by adjusting ε. (e),(f) Averaged fidelity for a Gaussian distribution of ε with variance $\sigma_\varepsilon^2 = \langle\varepsilon^2\rangle - \langle\varepsilon\rangle^2$. The maximization over time is done for the value $\varepsilon = \langle\varepsilon\rangle$ at the first (e) and fourth (f) local maximum.

and 3). We denote the time evolution according to a time-independent H_{eff} at time τ with $U_{\mathrm{eff}}(\tau)$ and consider the average gate fidelity [69]

$$F = \max_{\alpha} \frac{8 + |\mathrm{Tr}[e^{i\alpha\sigma_z} U_{\mathrm{eff}}(\tau) \mathrm{SWAP}^\dagger]|^2}{72}, \quad (3)$$

where we maximize over a z rotation in valley space, which is unimportant for the logical valley qubit in the singlet-triplet subspace. For the spin SWAP gate applied between dots I and II and between dots III and IV, the valley z rotation can be different. This difference is equivalent to a rotation of the S-T_0 valley qubit, which can be corrected afterwards. In the case $|A|, |B|, |C| \ll |\tilde{h}|$ considered here, we determine the phase α for the maximum in Eq. (3) analytically (see the Supplemental Material [67]). Figure 2 shows F for a detuning around $\varepsilon = \sqrt{U^2 - h^2}$, where the parameter $B = 0$. If furthermore C is negligible, we obtain $U_{\mathrm{eff}}(\tau_n) = \mathrm{SWAP}$ for $\varphi = \arccos n/(n+1)$ and $\tau_n = (n+1)\pi\hbar/A$. In Fig. 2, the situation is shown for $n = 0$ and $n = 3$. Figure 3 reveals that, also for other parameter regimes, $U_{\mathrm{eff}}(\tau)$ can be the spin SWAP gate with a high fidelity. The time τ where the maximal fidelity is reached is determined numerically. We include quasistatic charge noise, which was found to be important for GaAs DQDs [70], by averaging F over a Gaussian distribution of ε. We find that for the fluctuating bias ε with standard deviation $\sigma_\varepsilon = \sqrt{\langle\varepsilon^2\rangle - \langle\varepsilon\rangle^2} \approx \mu$eV the fidelity can be as high as $F \gtrsim 0.9999$ [see Figs. 2(e), 2(f), 3(e), and 3(f)]. We expect the noise sensitivity of $U_{\mathrm{eff}}(\tau)$ to be similar to exchange gates with spin DOF only (see the Supplemental Material [67]). Spin singlet-triplet qubits in silicon also suffer from

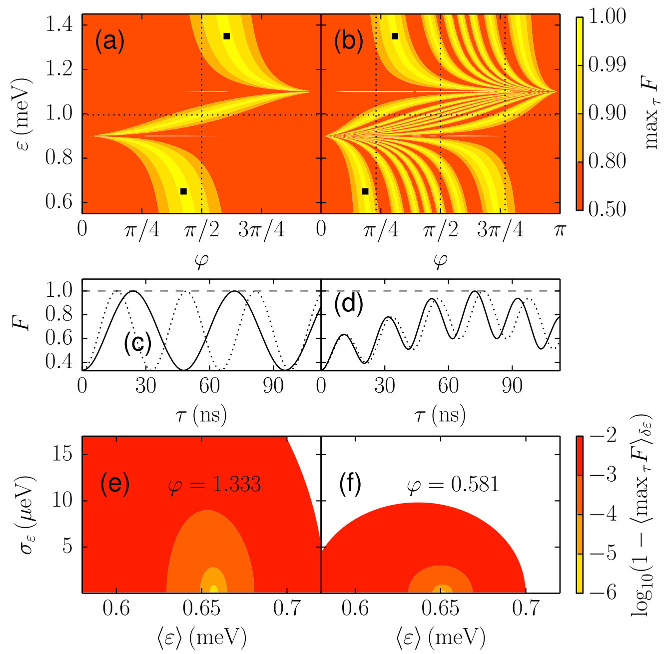

FIG. 3 (color online). Fidelity F for a broad range of the detuning ε and the phase φ in the hopping matrix elements, using the same parameters U, h, and t as in Fig. 2. (a),(b) F maximized over the gate time τ. We consider the first (a) and fourth (b) local maximum of F as a function of τ. The black squares indicate the positions in parameter space for the time-dependent plots (c),(d), namely, $\varepsilon = 1.35$ meV for the solid lines and $\varepsilon = 0.65$ meV for the dotted lines in (c),(d), $\varphi = 1.9$ (solid line), $\varphi = 1.333$ (dotted line) in (c), and $\varphi = 0.972$ (solid line), $\varphi = 0.581$ (dotted line) in (d). The horizontal dotted lines in (a),(b) represent $\varepsilon = \sqrt{U^2 - h^2}$, and the vertical dotted lines belong to values of φ being $\pi/2$ (a),(b) and $\arccos\frac{3}{4}$, $\pi - \arccos\frac{3}{4}$ (b). Note that the Schrieffer-Wolff transformation breaks down close to $\varepsilon = U \pm h$. (e),(f) Averaged fidelity for a Gaussian distribution of ε with $\sigma_\varepsilon^2 = \langle\varepsilon^2\rangle - \langle\varepsilon\rangle^2$. The maximum in time is determined for $\varepsilon = \langle\varepsilon\rangle$ at the first (e) and fourth (f) local maximum. The fidelity F is more robust at the first local maximum.

coupling to nuclear spins, but recent work concludes that charge noise is the dominating source of dephasing [71].

Hybrid quantum register.—Now we consider the entire register of n DQDs built in two different ways (Fig. 1) and prove that universal QC is possible in these two registers. It is sufficient to show that single-qubit gates for every qubit and a universal two-qubit gate between arbitrary qubits can be performed [72].

In the register Fig. 1(a), there is only one spin-only DQD, at position 1, and $(n-1)$ DQDs with spin and valley DOFs. Single-qubit gates for the qubits in the kth DQD, $1 < k \leq n$, can be performed by first transferring these qubits, both spin and valley, to DQD 2. This is done by applying $\mathrm{SWAP}_{\mathrm{spin}} \otimes \mathrm{SWAP}_{\mathrm{valley}}$ gates in the upper and the lower row of the register which allows interchanging the information of DQD k with $k-1$ and so on. The $\mathrm{SWAP}_{\mathrm{spin}} \otimes \mathrm{SWAP}_{\mathrm{valley}}$ gate is provided directly from the exchange interaction [14]. Second, the spin-only SWAP gate transfers the spin qubit into DQD 1, and in return the polarized ancilla spins into DQD 2. Now single-qubit operations can be performed for the spin S-T_0 qubit in DQD 1 and for the valley in DQD 2. The universal two-qubit gate between qubits in DQD k and in DQD m require transferring the qubits from these dots to DQDs 2 and 3. Then applying the spin-only SWAP moves the spin qubit from DQD 2 to DQD 1. The $\mathrm{SWAP}_{\mathrm{spin}} \otimes \mathrm{SWAP}_{\mathrm{valley}}$ gate between DQDs 2 and 3 and another spin-only SWAP yield a situation where the spin qubit from DQD k and the valley qubit from DQD m are together in DQD 2, where the universal two-qubit gate can be applied [14]. If two valley qubits or two spin qubits need to be involved in the two-qubit gate, the spin and the valley qubits can be interchanged when they are in DQD 2. The average number of additional SWAP gates needed for transferring qubits to the DQD at one end of the register before the desired gates can be applied is on the order of n^2 (see the Supplemental Material [67]). The register Fig. 1(b) contains a spin-only DQD for every spin-valley DQD. This allows for single-qubit operations without transferring qubits through the whole register. Two-qubit gates between arbitrary qubits can be performed, as spins can be moved within the entire register by spin-only SWAP gates. It is crucial to achieve high-fidelity spin-only and spin-valley SWAP gates. Errors in those operations can lead to leakage, as spin and valley could leave the singlet-triplet subspaces.

Materials.—We now focus on the materials which may provide the necessary properties for realizing our QC scheme. A natural choice seems to be a hybrid structure of one material without and one with a valley degeneracy where the hopping parameters t and φ across the interface can be controlled.

The sixfold valley degeneracy of bulk silicon is typically split off by a (001) interface [73–80]; the two lower valleys of interest, denoted $|z\rangle$ and $|\bar{z}\rangle$, are coupled by valley-orbit (VO) interaction, described by the complex matrix element V_{VO} [26]. In experiment, a valley splitting $2|V_{\mathrm{VO}}|$ in lateral silicon quantum dots of 0.1–1 meV has been reported [39–46]. Electrical tunability in the range from 0.3 to 0.8 meV was demonstrated [45]. Calculations show that, while $\arg(V_{\mathrm{VO}})$ is only slightly influenced by an applied electric field [61], it depends on the conduction band offset [29]; thus, a structure with an alternating top layer material, e.g., SiO_2 and SiGe or $Si_{1-x}Ge_x$with a varying x could provide the difference in $\arg(V_{\mathrm{VO}})$, i.e., $\varphi \neq 0$, which is needed in our scheme between dots I and II and between III and IV, while $\arg(V_{\mathrm{VO}})$ should be the same in dots II and IV. Whereas the band offset difference is higher between Si/SiO_2 and Si/SiGe, charge traps at the Si/SiO_2 interface can be a source for noise [81]; nevertheless, spin blockade was demonstrated in Si/SiO_2 structures with a reduced density of traps [82]. Furthermore, one requires a large valley splitting in dots I and III, which results in a situation where effectively only one valley state participates in the dynamics.

Graphene provides a twofold valley degeneracy and should allow for a two-dimensional array of quantum dots. Theory shows that the valley state is affected by a magnetic field perpendicular to the graphene plane [65] and in graphene nanoribbons also by the boundary conditions [54].

Dual hybrid register.—Interchanging the roles of spin and valley yields DQDs with spin and valley DOF and with valley DOF only. A strong local magnetic field could yield conditions where only the lowest spin states in this DQD have to be taken into account; the spin Zeeman splitting has to be large compared to the exchange interaction, e.g., 0.01 meV in Ref. [3]. To achieve a different phase between these spin states and the spins of the energy eigenstates in the spin-valley dots, the direction of the magnetic field has to be different for different dots. Therefore, this alternative approach seems to have less stringent requirements from the material point of view (phase of valley states can be the same) but would require a field gradient of several Teslas on a nanometer scale.

Conclusion.—In conclusion, we have shown that combining spin and valley singlet-triplet qubits allows for a new hybrid spin-valley QC scheme. Necessary conditions are control over the Zeeman splitting for spin and valley as well as over the phase of the valley states, the realization of high-fidelity SWAP operations, and long enough valley coherence times. The concept relies crucially on the controlled coexistence of spin and valley qubits allowing for universal QC based on the electrically tunable exchange interaction.

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