Light-Hole Gate-Defined Spin-Orbit Qubit

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The selective confinement of light-holes (LHs) is demonstrated by introducing a low-dimensional system consisting of highly tensile-strained Ge quantum well enabling the design of an ultrafast gate-defined spin qubit under the electric dipole spin resonance. The qubit size-dependent $g$-factor and dipole moment are mapped, and the parameters inducing their modulation are discussed. It is found that the LH qubit dipole moment is 2 to 3 orders of magnitude higher than that of the canonical heavy-hole qubit. This behavior originates from the significant spin splitting resulting from the combined action of large cubic and linear Rashba spin-orbit interactions that are peculiar to LHs. The qubit relaxation rate is also affected by the strong spin-orbit interaction and follows typically a $B^2$ behavior. The proposed all-group IV, direct bandgap LH qubit provides an effective platform for a scalable qubit-optical photon interface sought-after for long-range entanglement distribution and quantum networks.

Gated quantum dots (QDs) exploiting the strong spin-orbit interaction (SOI) of holes and their quiet quantum environment provide practical building blocks for quantum processors \cite{1,11}. However, due to the restricted choice of low-dimensional systems (e.g., Ge/SeGe), current hole spin qubits are based predominately on heavy-hole (HH) spins \cite{12}. Notwithstanding this progress, the ability to utilize light-hole (LH) spins would enable additional degrees of freedom to engineer qubits with extended functionalities. Indeed, LHs allow simple schemes for a direct mapping of superposition from a flying qubit to a stationary spin qubit \cite{14} as well as a better resilience against charge noise \cite{14} and an enhanced proximity-induced superconductivity transfer \cite{15}. Additionally, LHs are also known to have strong SOI yielding fast Rabi oscillations \cite{14}. Nevertheless, the development of LH qubits has been hampered by the lack of proper material systems. Here, we address this limitation and introduce a new low-dimensional system to control LH states.

The selective confinement of LHs in Ge quantum well (QW) requires sufficiently high tensile strain, which can be achieved using the emerging germanium-tin (Ge$_{1-x}$Sn$_x$) alloys \cite{10}. Ge/Ge$_{1-x}$Sn$_x$ hole spin devices combine all advantages that are inherent to group IV semiconductors \cite{17,18}. Besides the weaker hyperfine interaction with the surrounding nuclear spin bath resulting from the $p$-symmetry of the hole wavefunction \cite{19,21}, the strong SOI in the valence band of Ge and Sn would enable all-electrical driving of the qubit without the need for an external RF transmission line and create rich spin-related phenomena unique to holes \cite{22,23}. Moreover, the Ge$_{1-x}$Sn$_x$ alloy spans a wide range of lattice parameters \cite{24,20}, which is useful to control the hole spin properties through the epitaxial strain directly on silicon wafers \cite{16,27,28}.

Fig. 1 illustrates the gate-defined LH QD. Note that the lattice mismatch between Ge and Ge$_{1-x}$Sn$_x$ induces a significant tensile strain in the Ge layer, which lifts the HH-LH degeneracy yielding a LH-like valence band edge (Fig 1b). The Ge$_{1-x}$Sn$_x$/Ge/Ge$_{1-x}$Sn$_x$ heterostructure confines LHs in the Ge layer for $x$ typically higher than 0.11, while the HHs are pulled into the Ge$_{1-x}$Sn$_x$ barriers \cite{16}. A set of electrostatic gates on top of the heterostructure helps confine the LH in the plane by applying a DC voltage. Note that Ge becomes a direct bandgap semiconductor at a tensile strain higher than 1.8%. The EDSR is performed by applying a microwave voltage. A feature that is sometimes neglected \cite{29,31} but needs to be accounted for in this system is the spread of the LH wavefunction into the barriers. Because the LHs are located in the barriers, LH-HH mixing wavefunction overlap only occurs outside the QW. Assuming a hard wall potential at the interface is therefore equivalent to neglecting entirely the LH-HH mixing. Moreover, the LH subband dispersion non-parabolicity must also be considered. The theoretical framework below for the in-plane motion of the LHs explicitly takes into account these peculiar features.

Eight-band $k \cdot p$ theory \cite{33} is used for the derivation of an effective Hamiltonian for the 2D LH gas incorporating the Bir-Pikus Hamiltonian and thus the effects of bi-axial epitaxial strain \cite{24}. [001]-oriented substrates are considered, with the growth direction parallel to the $z$-axis. The operator ordering between material parameters and wavevector components require special care to avoid spurious solutions and to properly include the effects of an external magnetic field \cite{35,30}. An out-of-plane magnetic field $B = B e_z$ results in the following commutation relations for the mechanical wavevector components: $[K_\alpha, K_\beta] = \epsilon_{\alpha\beta\gamma} z i \lambda^2$, where $\epsilon$ is the Levi-Civita tensor, $\lambda = \sqrt{\hbar/eB}$ is the magnetic length and $\alpha, \beta = \{x, y, z\}$. The mechanical wavevector $K = k + \epsilon A / \hbar$ is given in terms of the canonical wavevector $k \rightarrow -i \nabla$. In the symmetric gauge, the vector potential $A = B/2(-ye_x + xe_y)$.

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The total Hamiltonian $H_\parallel$ for the in-plane motion of holes and electrons is written as a sum of different contributions [30]:

$$H_\parallel = H_{k\cdot p}K_\parallel + V(z),$$

where $K_\parallel = K_x e_x + K_y e_y$, $H_{k\cdot p}$ is the eight-band $k\cdot p$ matrix including strain and magnetic effects [33, 36, 37] and $V(z)$ is the band alignment. This last term also includes the effects of an out-of-plane electric field $E = E_z e_z$.

The first step to find an effective LH Hamiltonian is to calculate the envelope functions and energies of $H_\parallel$ at $K_x = K_y = 0$ and $B = 0$. This provides an orthonormal basis (a set of subband edges) on which $H_\parallel$ is projected at finite $K_\parallel$ and $B > 0$. This orthonormal basis contains two types of subbands. The first are pure HH subbands (H subbands) and the second are superpositions of LH, SO holes, and CB electrons ($\eta$ subbands):

\begin{align}
|H; l, \sigma\rangle &= \frac{3}{2} \frac{3\sigma}{2} |l\rangle_h, \\
|\eta; j, \sigma\rangle &= \left( \frac{1}{2} \frac{\sigma}{2} \right)_c |j\rangle_c + \left( \frac{3}{2} \frac{\sigma}{2} \right)_s |j\rangle_s,
\end{align}

where $l$ and $j$ are respectively the subband indices for $H$ and $\eta$ subbands and $\sigma = \pm 1$ is the pseudo-spin index. The first ket in each term represents bulk Bloch functions at the $\Gamma$ point, while the second ket represents the envelope functions. The labels $h, c, s$ refer to the HH, CB, LH and SO part of the spinor, respectively. Because subbands are either of type $H$ or $\eta$, a “LH” subband is understood as an $\eta$ subband such that $\langle j | j \rangle_c > \langle j | j \rangle_s$ and $\langle j | j \rangle_s > \langle j | j \rangle_s$. Following the projection of $H_\parallel$ upon the basis $\{|\eta\rangle, |H\rangle\}$, a 4th order Schrieffer-Wolff transformation [38] is applied leading to an effective Hamiltonian for $\eta$ subbands:

$$H_{\text{eff}} = \alpha_0 \tilde{\gamma} K^2 + \alpha_0 \tilde{g} \gamma_{\text{SO}} + \alpha_0 \gamma_{\text{eff}} K^2 + \alpha_0 \gamma_{\text{SO}} K^2$$

with $\alpha_0 = h^2/(2m_0)$, $m_0$ the free electron mass, $K_\pm = K_x \pm i K_y$, $\gamma_{\text{SO}} = (\gamma_{\text{SO}} + i \gamma_{\text{eff}})/2$ and $\gamma_{\text{SO},\pm}$ the Pauli matrices. The first term in [2] corresponds to the parabolic contribution in the dispersion relation, with $\tilde{\gamma}$ the effective mass parameter. The second term corresponds to the linear Zeeman splitting, with $\tilde{g}$ the effective $g$-factor. The next three terms correspond to non-parabolicity ($\tilde{\gamma}'$), Zeeman splitting non-linearity ($\tilde{g}'$), and a hybrid term proportional to $K^2/\lambda^2$. The band structure anisotropy is taken into account by the $\gamma$ parameter. Finally, the last three terms correspond to the linear Rashba splitting ($\beta_1$) and two kinds of cubic Rashba splitting ($\beta_2$ and $\beta_3$). The effective parameters in [2] in terms of the envelopes $|l\rangle_k$ and $|j\rangle_{c,t,s}$ are presented in [37]. This approach is similar to that employed by [26, 31] for instance. However, here the spread of the wavefunction into the barriers and the effects of $E$ are implicitly taken into account from the shape of the envelopes, and the effective parameters in [2] are calculated from a larger subband edge basis due to the large amount of HH levels in the barriers. Fig. 1 shows the dispersion of the ground LH subband for two different QWs. Fig. 1(c) displays the case of a 13 nm Ge QW with relaxed Ge$_{0.85}$Sn$_{0.15}$ barriers.
The QD Hamiltonian includes the isotropic and parabolic confinement from the top gates: $H_{\text{QD}} = H_{\text{eff}} + m^* \omega_0^2 (x^2 + y^2)/2$, where $m^* = m_0/\gamma$ is the in-plane effective mass. $H_{\text{QD}}$ is diagonalized by first writing $H_{\text{QD}} = H_0 + H'$, where $H_0$ consists of the first two terms in (2) plus the parabolic confinement:

$$H_0 = \alpha_0 \gamma K_\parallel^2 + \frac{1}{2} m^* \omega_0^2 (x^2 + y^2) + \frac{\alpha_0 \beta}{\lambda^2} \sigma_z. \quad (3)$$

$$= \hbar \omega_l \left(a_1^\dagger a_1 + a_2^\dagger a_2 + 1\right) + \frac{\hbar \omega_c}{2} \left(a_1^\dagger a_1 - a_2^\dagger a_2\right) + \frac{\alpha_0 \beta}{\lambda^2} \sigma_z, \quad (4)$$

where

$$a_1 = \frac{x - iy}{2r} + \frac{ik_-}{2}, \quad a_2 = \frac{x + iy}{2r} + \frac{ik_+}{2}. \quad (5)$$

are ladder operators, $k_\pm = k_x \pm ik_y$, $\omega_c = eB/m^*$, $\omega_l^2 = \omega_0^2 + \omega_c^2/4$ and $r = \sqrt{\hbar/(m^* \omega_0)}$ is the effective quantum dot radius. The eigenstates of $H_0$, the so-called Fock-Darwin orbitals $|n_1, n_2, \sigma\rangle$ with $n_{1,2} = 0, 1, \ldots$ and $\sigma = \pm 1$, provide an orthonormal basis on which $H_{\text{QD}}$ is projected. The eigenvalues of the resulting matrix for $H_{\text{QD}}$ in the Fock-Darwin basis are then solved numerically. The two lowest energy orbitals $|0\rangle$ and $|1\rangle$ corresponding to energies $E_0$ and $E_1$ define the qubit. These are mostly composed of the Fock-Darwin orbitals $|0, 0, -\rangle$ and $|0, 0, +\rangle$, respectively, plus higher-energy orbitals:

$$|0\rangle = |0, 0, -\rangle + \left(c_{0,1}^{(0)} |0, 1\rangle + c_{3,0}^{(2)} |3, 0\rangle + c_{1,2}^{(0)} |1, 2\rangle\right) |+\rangle \quad (6a)$$

$$|1\rangle = |0, 0, +\rangle + \left(c_{1,0}^{(0)} |1, 0\rangle + c_{0,3}^{(2)} |0, 3\rangle + c_{2,1}^{(2)} |2, 1\rangle\right) |\rangle. \quad (6b)$$

The coefficients $c_{n_1, n_2}^{(i)}$ were extracted from the numerical diagonalization of $H_{\text{QD}}$ to avoid artifacts near crossings between Fock-Darwin orbitals. They can be evaluated with perturbation theory away from these crossings [37].

For a driving field $E(t) = E_\text{AC} \cos(\omega t)$, where $\hbar \omega = |E_\text{AC} - E_\text{q}|$ is the qubit energy, the Rabi frequency $\Omega$ is given in terms of the qubit dipole moment $d = \langle 0 | x | 1 \rangle$ by $\Omega = E_\text{AC} d/\hbar$.

Fig. 2 shows the QD orbital energies as a function of the QD radius $r_q = \sqrt{\hbar/m^* \omega_0} = 25$ nm and the same QW parameters as in Fig. 1. The qubit undergoes a transition from a spin qubit to a charge qubit at the crossing between $|1\rangle$ and the mostly $|0, 1, -\rangle$ orbital near $B = 0.275$ T. The two levels cross because $|0, 1, -\rangle$ is not present in the expansion of $|1\rangle$. The qubit dipole moment $d$ and the qubit $g$-factor $|g_{\text{QD}}|$ are plotted in Fig. 3 as a function of the QD radius $r_q$ and
$B = 0.05$ T. The $g$-factor has a strong dependence on $r_0$ for small radii, and approaches asymptotically the QW value $\bar{g} = 8.69$ at large $r_0$. The large $\bar{g}$ value originates from the first order approximation $\bar{g} \approx 2\kappa$ for a LH spin in a perpendicular magnetic field with $\kappa = 3.41$ in Ge. Deviations from $2\kappa$ come from the spread of the wavefunction and 2nd order corrections [37, 42]. The dipole moment $d$ takes very large values for two main reasons. First, the coefficient $\beta_2$ that contributes to EDSR by introducing a $|1, 0, −⟩$ contribution into $|1⟩$ depends on the sum $(\gamma_2 + \gamma_3)$ for LHs [37] whereas for HHs it depends on the difference $(\gamma_2 − \gamma_3)$. In Ge, $\gamma_2 \approx \gamma_3$ [43] and therefore $\beta_3$ is much larger for LHs. Secondly, LHs are subject to a linear Rashba spin splitting proportional to $\beta_1$, which is non-existent for HHs. This additional term contributes to a large $d$ similarly to $\beta_3$ by increasing the contribution of $|1, 0, −⟩$ into $|1⟩$. At $≈ 27.5$ nm, $|d|$ reaches a maximum as a result of the combined effects of $\beta_1$ and $\beta_3$, which gives a dipole moment that is $2$ to $3$ orders of magnitude larger than that of HHs in a compressively strained Ge [29, 44]. For instance, an in-plane driving field as small as $E_{AC} = 1$ mV/µm gives a Rabi frequency $\Omega \approx 1.2$ GHz.

There is, however, a range of QD radii where the dipole moment is very small (Fig. 3). This happens because both $\beta_1$ and $\beta_3$ contribute to $d$. When $B$ is small such that $|1⟩$ is far from the excited orbitals, the dipole moment is given by

$$|d| \approx \frac{e m^* r^2 |\bar{g}| \mu_B B}{\hbar^2} \left|r^2 \beta_1 + 2 \beta_3\right|.$$  \hspace{1cm} (7)

Therefore, when $\beta_1 \beta_3 < 0$, $d$ can vanish at specific values of $r_0$ and $B$. For the QW parameters in Fig. 1, $\beta_1 = 0.42$ meV nm and $\beta_3 = −290$ meV nm$^3$ which causes the dipole moment to vanish at $B = 0.05$ T and $r_0 \approx 37$ nm. For $r_0 > 37$ nm $d$ increases again, but at the cost of a smaller orbital energy spacing.

An important feature of LH qubits is that EDSR is driven by both $\eta$-H and $\eta$-$\eta$ mixing. This is because there is an allowed 1st order coupling between $\eta$ subbands $⟨\eta; j| H' |\eta; j', −⟩ = R_{j,j'}K_−$ that is nonexistent for HHs [37]. The $\eta$-$\eta$ mixing part contributes mainly to the $\beta_3$ parameter through a term proportional to $(\gamma_2 + \gamma_3)$, while $\eta$-$\eta$ mixing contributes to both $\beta_3$ and $\beta_1$. Notably, these two types of mixing are of equal importance given that $\beta_1$ and $\beta_3$ can interfere to suppress the dipole moment (c.f. [1]).

The relaxation time $T_1 = 1/\Gamma$ of the LH qubit was also evaluated for the system in Fig. 1. The coupling of the hole to acoustic phonons was considered. The total relaxation rate $\Gamma = \Gamma_{em} + \Gamma_{abs}$, where $\Gamma_{em}$ ($\Gamma_{abs}$) is the rate associated with the emission (absorption) of one phonon. Each of these rates is calculated by Fermi’s golden rule:

$$\Gamma_i = \frac{2\pi V}{\hbar} \sum_\alpha \int \frac{d^3 q}{8\pi^3} |\langle f | W_\alpha | i \rangle|^2 \delta(\hbar\omega − \hbar\omega_{\alpha q}),$$  \hspace{1cm} (8)

where $V$ is the volume of the system and $\hbar\omega_{\alpha q} = \hbar v_{\alpha q}$ is the phonon energy in branch $\alpha = \{LA,TA1,TA2\}$ and with momentum $q = q_\alpha$. $|i,f⟩$ represent initial and final qubit levels upon absorption or emission of a phonon. The operator $W_\alpha$ is derived from the hole-phonon Hamiltonian in a procedure similar to that in [31, 45, 47]. See [37] for details. Importantly, the matrix element $⟨f | W_\alpha | i⟩$ takes into account the relaxation rate associated with all three spin-orbit parameters $\beta_1$, $\beta_2$, and

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3}
\caption{LH qubit dipole moment (left) and absolute value of the $g$-factor (right) as a function of the QD radius $r_0$. The magnetic field is fixed at 0.05 T. The QW parameters are the same as in Fig. 1.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4}
\caption{Relaxation rate $\Gamma = 1/T_1$ as a function of the magnetic field. The QW parameters are the same as in Fig. 1.}
\end{figure}
$
abla \beta_3$.

Fig. 4 shows the computed $\Gamma$ as a function of $B$ for the Ge/GeSn QW system in Fig. 4 at $r_0 = 25 \text{ nm}$. A relaxation time $T_1 = 100 \mu s$ was extracted at $B = 0.1 \text{ T}$. Moreover, $\Gamma$ follows a $B^7$ behavior when $B \gg \sqrt{2k_B T/(g_{QD} \mu_B)}$ and a $B^6$ behavior when $B \ll \sqrt{2k_B T/(g_{QD} \mu_B)}$. This higher relaxation rate for LHs compared to HHs [12, 91] is due to the larger spin-orbit coupling parameters $\beta_{1,2,3}$. The $B^7$ behavior at low temperature is associated to the spin-orbit term $|r^2(\beta_1 + 2\beta_3)|$ that was encountered in eq. (7) and from the sum $c_{0,1}^{(2)} + c_{1,0}^{(1)} \sim B$.

Similar calculations were also performed at a QD radius $r_0 = 37.9 \text{ nm}$ for which the dipole moment vanishes at $B = 0.05 \text{ T}$ (Fig. 4). In this case, two different regimes were observed: for $B \ll 0.05 \text{ T}$ the relaxation rate exhibits a $B^7$ behavior, but at $B \ll 0.05 \text{ T}$ it evolves as $\sim B^{11}$. This is because the term associated with $|r^2(\beta_1 + 2\beta_3)|$ vanishes and the dominating terms in $\Gamma$ are those associated with $\beta_2$, $\beta_3$ alone and the superposition coefficients $c_{n_1,n_2}^{(0,1)}$ with $n_1 + n_2 = 3$. At $B = 0.1 \text{ T}$, $T_1 = 8 \text{ ms}$, which is consistent with a much smaller dipole moment at this radius. The abrupt change in behavior around $B = 0.14 \text{ T}$ is due to a very small anti-crossing between $|1\rangle$ and the mostly $|1,0,-\rangle$ orbital, while at $B = 0.5 \text{ T}$ it is caused by a small anti-crossing between the mostly $|1,0,-\rangle$ and the mostly $|0,3,-\rangle$ orbital.

In conclusion, this work unravels the spin properties of a light-hole gated quantum dot in tensile strained Ge under EDSR. A detailed framework is described taking into account the spread of the envelopes in the barriers surrounding the quantum well and the effects of the dispersion non-parabolicity. It was found that light-holes have a large cubic Rashba parameter ($\beta_3$) and the existence of a non-zero linear Rashba parameter ($\beta_1$). Interestingly, $\beta_1$ and $\beta_3$ can interfere destructively and cause the dipole moment to vanish at a specific quantum dot size. The relaxation rate $\Gamma$ of a light hole qubit follows a $B^7$ behavior, except when $d \approx 0$ where $\Gamma$ follows a $B^{11}$ behavior. This direct bandgap Ge/GeSn device structure provides additional degrees of freedom to implement silicon-compatible and scalable quantum processors leveraging the advantages of light-hole spin properties in addition to their efficient coupling with optical photons and their ability to transfer superconductivity.

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