Spin decoherence of a heavy hole coupled to nuclear spins in a quantum dot

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We theoretically study the interaction of a heavy hole with nuclear spins in a quasi-two-dimensional III-V semiconductor quantum dot and the resulting dephasing of heavy-hole spin states. It has frequently been stated in the literature that heavy holes have a negligible interaction with nuclear spins. We show that this is not the case. In contrast, the interaction can be rather strong and will be the dominant source of decoherence in some cases. We also show that for unstrained quantum dots the form of the interaction is Ising-like, resulting in unique and interesting decoherence properties, which might provide a crucial advantage to using dot-confined hole spins for quantum information processing, as compared to electron spins.

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I. INTRODUCTION

The spin of a quantum-dot-confined electron is considered a major candidate for the realization of solid-state-based quantum bits, the basic building blocks for quantum information processing devices and, eventually, for a quantum computer.1 One of the main obstacles to building these devices is the decay of spin coherence. The ultimate limit to the coherence time for electron spins in most quantum dots at low temperatures is set by the hyperfine interaction with nuclei in the host material.2,3,4,5

If no special effort is made to control this environment, the associated coherence times are quite short, typically on the order of nanoseconds.2,3,4,5

Very recently, several experiments have shown initialization and readout of single hole spins in self-assembled quantum dots,6,7,8,9 and control over the number of holes in single gated quantum dots.10,11 Prerequisites for single-hole-spin dephasing-time measurements. Ensemble hole-spin dephasing times have recently been measured in p-doped quantum wells.12 Hole-spin coherence times in III-V semiconductor quantum dots are anticipated to be much longer than electron-spin coherence times due to a weak hyperfine coupling relative to conduction-band electrons.13,14,15,16,17,18,19,20,21 In the present work, we show that, in contrast, the coupling of a heavy hole (HH) to the nuclear spins in a quantum dot can be rather strong, potentially leading to coherence times that are comparable to those for electrons. However, in the quasi-two-dimensional (Q2D) limit, this interaction takes-on a simple Ising-like form,

\[ H = \sum_k A_k^h s_z I_z, \]  

where \( A_k^h \) is the coupling of the HH to the \( k \)th nucleus, \( s_z \) is the hole pseudospin-\( \frac{1}{2} \) operator, and \( I_z \) is the \( z \)-component of the \( k \)th nuclear-spin operator \( I_k \). The form of this effective Hamiltonian has profound consequences for the spin dynamics. Coherence times can be

dramatically extended by preparing the slowly-varying nuclear field in a well-defined state ("narrowing" the field distribution)6,22,23,24,25,26,27. For an electron spin interacting with nuclei via the contact hyperfine interaction, narrowing is effective only up to the time scale where slow internal nuclear-spin dynamics or transverse-coupling ("flip-flop") terms become relevant. Here we will show that heavy holes confined to two dimensions have negligible flip-flops, potentially leading to significantly longer spin coherence times. The strong coupling of the HH to the nuclear spins is not due to confinement but is also present in bulk crystals, while the Ising-like interaction is a feature of Q2D systems.

This paper is organized as follows: In Sec. II we write down the nuclear-spin interactions and derive an effective spin Hamiltonian for a quantum-dot-confined HH. In Sec. III we calculate the dynamics of the transverse HH spin for different external magnetic field directions. In Sec. IV we give estimates of the coupling strengths for the special case of a GaAs quantum dot. Conclusions and comparison to recent experiments can be found in Sec. V. Technical details are deferred to Appendices A–D.

II. NUCLEAR-SPIN INTERACTIONS

A. Hamiltonians

For a relativistic electron in the electromagnetic field of a nucleus with non-zero spin at position \( \mathbf{R}_k \), there are three terms that couple the electron spin and orbital angular momentum to the spin of the nucleus: the Fermi contact hyperfine interaction \( h^A_1 \), a dipole-dipole-like interaction (the anisotropic hyperfine interaction, \( h^A_2 \)), and the coupling of electron orbital angular momentum to the nuclear spin \( \hbar \). Setting \( \hbar = 1 \), these interactions are...
described by the following Hamiltonians:25

\[

d_1^k = \frac{\mu_0}{4\pi} \frac{8\pi}{3} \gamma_S \gamma_{jk} \delta(r_k) \mathbf{S} \cdot \mathbf{I}_k, \quad (2)
\]

\[

d_2^k = \frac{\mu_0}{4\pi} \gamma_S \gamma_{jk} \frac{3(\mathbf{n}_k \cdot \mathbf{S})(\mathbf{n}_k \cdot \mathbf{I}_k) - \mathbf{S} \cdot \mathbf{I}_k}{r_k^2(1 + d/r_k)}, \quad (3)
\]

\[

d_3^k = \frac{\mu_0}{4\pi} \gamma_S \gamma_{jk} \frac{\mathbf{L}_k \cdot \mathbf{I}_k}{r_k^2(1 + d/r_k)}. \quad (4)
\]

Here, \(\gamma_S = 2\mu_B\), \(\gamma_{jk} = g_k \mu_N\), \(\mu_B\) is the Bohr magneton, \(g_k\) is the nuclear \(g\)-factor of isotopic species \(j_k\), \(\mu_N\) is the nuclear magneton, \(r_k = r - R_k\) is the electron-spin position operator relative to the nucleus, \(d \approx Z \times 1.5 \times 10^{-15} \text{ m}\) is a length of nuclear dimensions, \(Z\) is the charge of the nucleus, and \(\mathbf{n}_k = r_k/r_k\). \(\mathbf{S}\) and \(\mathbf{L}_k = r_k \times \mathbf{p}\) denote the spin and orbital angular-momentum operators of the electron, respectively.

Nuclear-spin interactions are typically much weaker than the spin-orbit interaction. It is therefore appropriate to form effective Hamiltonians with respect to a basis of eigenstates of the Coulomb and spin-orbit interactions. The 8 \times 8 Kane Hamiltonian, which describes the band structure of a III-V semiconductor, provides such a basis.23,24 The Kane Hamiltonian is usually written in terms of conduction-band (CB) and valence-band (consisting of HH, light-hole (LH), and split-off sub-band) states. We derive an approximate basis of eigenstates in the HH sub-band by projecting the 8 \times 8 Kane Hamiltonian onto the two-dimensional HH subspace.

To form effective Hamiltonians, we must approximate the crystal-Hamiltonian eigenfunctions given by Bloch’s theorem for a single band \(n\): \(\Psi_{n\mathbf{k}\sigma}(r) = \frac{1}{\sqrt{N_A}} \exp(i \mathbf{k} \cdot \mathbf{r}) u_{n\mathbf{k}\sigma}(r)\), where \(N_A\) is the number of atomic sites in the crystal, and the Bloch amplitudes \(u_{n\mathbf{k}\sigma}(r)\) have the periodicity of the lattice.

We will approximate the \(k = 0\) Bloch amplitudes \(u_{n\mathbf{0}\sigma}(r)\) within a primitive unit cell by a linear combination of atomic orbitals (see Eq. 12, below). Near an atomic site, the CB Bloch amplitudes have approximate \(s\)-symmetry (angular momentum \(l = 0\)), whereas the HH and LH Bloch amplitudes have approximate \(p\)-symmetry \((l = 1\)). Adding spin, the \(s\)-component of total angular momentum of a HH is \(m_J = \pm 3/2\), whereas a LH has \(m_J = \pm 1/2\). In the Q2D limit, i.e., going from the bulk crystal to a quantum well (whose growth direction we take to be [001]), a splitting \(\Delta_{\text{LH}}\) develops between the HH and LH sub-bands at \(k = 0\). We estimate \(\Delta_{\text{LH}} \simeq 100\, \text{meV}\) for a quantum well of height \(a_s \simeq 5\, \text{nm}\) in GaAs, much larger than the hyperfine coupling (see Appendix A). The splitting \(\Delta_{\text{LH}}\) is essential since it produces a well-defined two-level system in the HH sub-band, and we can restrict our considerations to the manifold of \(m_J = \pm 3/2\) states.

B. Interactions in an atom

Before addressing confinement in quantum dots, we illustrate that the interaction of an electron in a hydrogenic \(p\) orbital with the spin of the nucleus (which we choose to be at \(R_k = 0\)) is generally non-zero. Moreover, when projected onto the manifold of \(m_J = \pm 3/2\) states, this interaction takes-on a simple Ising form. Although our final analysis will apply to any III-V semiconductor, we will take GaAs as a concrete example.

The effective screened nuclear charges \(Z_{\text{eff}}\) “felt” by the valence electrons (in 4s and 4p orbitals) in Ga and As atoms have been calculated in Ref. 31. The 4s orbitals and 4p orbitals (with orbital angular momentum \(m_L = \pm 1\)) are given in terms of hydrogenic eigenfunctions with the replacements \(Z \rightarrow Z_{\text{eff}}\) by \(\Psi_{400}(r) = R_{40}(r)Y_{00}^{0}(\theta, \varphi)\) and \(\Psi_{41\pm 1}(r) = R_{41}(r)Y_{1\pm 1}^{0}(\theta, \varphi)\), respectively. Including spin and evaluating matrix elements of the Hamiltonians 22-41 with respect to hydrogenic 4s states leads to effective spin Hamiltonians of the form 22-41 \(h^{4s}_{\text{eff}} = A_s \mathbf{S} \cdot \mathbf{I}_k\) and, due to the spherical symmetry of the wavefunction, \(h^{4p}_{\text{eff}} = h^{4s}_{\text{eff}} = 0\). The same procedure with the 4p states leads to effective Hamiltonians \(h^{4p}_{\text{eff}} = 0\) (since \(p\)-states vanish at the origin) and \(h^{4p}_{\text{eff}} + h^{4s}_{\text{eff}} = A_s s_z I_z\), where \(s_z = \pm \frac{1}{2}\) corresponds to \(m_J = \pm 3/2\). \(A_s\) and \(A_p\) denote the coupling strengths of electrons in 4s and 4p orbitals, respectively. Evaluating all integrals exactly gives \(A_p/A_s = 1/5\ (Z_{\text{eff}}(\kappa, 4p)/Z_{\text{eff}}(\kappa, 4s))^3\), \(\kappa = \text{Ga, As}\).

Quite significantly, after inserting values of \(Z_{\text{eff}}\) from Ref. 31 into Eq. 8, we find that the ratio of coupling strengths is fairly large – on the order of 10%: \(A_p/A_s \simeq 0.14\) for Ga, and \(A_p/A_s \simeq 0.11\) for As. Since \(h^{4p}_{\text{eff}}\) and \(h^{4s}_{\text{eff}}\) do not contribute to the hyperfine interaction of an electron in an \(s\) orbital, research on hyperfine interaction for electrons in an \(s\)-type conduction band has focused on the contact term \(h^{4s}_{\text{eff}}\), neglecting the other interactions. The fact that \(h^{4s}_{\text{eff}}\), in contrast, gives no contribution for an electron in a \(p\) orbital has led to the claim that electrons in \(p\) orbitals (and holes) do not interact with nuclear spins. Eq. 10 shows that \(h^{4s}_{\text{eff}}\) and \(h^{4p}_{\text{eff}}\) can contribute significantly. Furthermore, while the interaction of a 4s-electron with the nuclear spin is of Heisenberg type, within the manifold of \(m_J = \pm 3/2\) states, the interaction of a 4p-electron is Ising-like at leading order (virtual transitions via the \(m_J = \pm 1/2\) states may lead to non-Ising corrections). This result is a direct consequence of the Wigner-Eckart theorem and the fact that the Hamiltonians 22-41 can be written in the form \(h^{4s}_{\text{eff}} = \mathbf{v}_s^k \cdot \mathbf{I}_k\), where \(\mathbf{v}_s^k\) are vector operators in the electron (spin and orbital) Hilbert space.
C. Interactions in a quantum dot

We now return to the problem directly relevant to a HH in a two-dimensional quantum well. We consider an additional circular-symmetric parabolic confining potential in the plane of the quantum well defining a quantum dot. Neglecting hybridization with other bands, which we estimate to be typically on the order of 1% (see Appendix A), the pseudospin states for a HH within the envelope-function approximation read \(|\Psi_\sigma\rangle = |\phi; u_{\text{HH},\sigma}\rangle |\sigma\rangle\), where |\phi; u_{\text{HH},\sigma}\rangle and |\sigma\rangle (\sigma = \pm) denote the orbital and spin states, respectively. The orbital wavefunctions are given explicitly by |\phi; u_{\text{HH},\sigma}\rangle = \sqrt{v_0} \phi(r) u_{\text{HH},\sigma}(r)\). Here, \(v_0\) is the volume occupied by a single atom (half the volume of a two-atom zinc-blende primitive unit cell), and \(\phi(r) = \phi_\sigma(z) \phi_\rho(\rho)\) is the envelope function. The radial ground-state envelope function is a Gaussian:

\[
\phi_\rho(\rho) = \frac{1}{\sqrt{\pi \rho}} \exp \left( -\frac{\rho^2}{2\rho_0^2} \right),
\]

where \(\rho = (x,y)\), \(\rho = |\rho|\), \(l_0 = l_0 [1 + (B_z/B_0)^2]^{-1/4}\), \(B_z\) is the component of an externally applied magnetic field along the growth direction and \(B_0 = \Phi_0/\pi \rho_0^2\) where \(\Phi_0 = \hbar/|e|\) is a flux quantum. A typical dot Bohr radius of \(l_0 = 30\, \text{nm}\) gives \(B_0 \approx 1.5\, \text{T}\).

In a solid, the HH is delocalized over the lattice sites of the crystal. The nuclei do not interact solely with the fraction of the HH in the same primitive unit cell (‘on-site’ interaction), but also with density localized at more distant atomic sites (long-ranged interactions). We neglect the long-ranged interactions, which lead to corrections on the order of 1% relative to the on-site interaction (see Appendix B). If the envelope function varies slowly on the length scale of a primitive cell, we find (combining \(h_z^2\) and \(h_y^2\)) \(A_k^b = A_k^b v_0 |\phi(R_k)|^2\), where

\[
A_k^b = -\frac{\mu_0}{4\pi} \gamma_g \gamma_j \left< \frac{3 \cos^2 \theta_k + 1}{r_k^2 (1 + d/r_k)} \right>_{\text{p.e.}}.
\]

Here, \(<\cdots>_{\text{p.e.}}\) denotes the expectation value with respect to \(u_{\text{HH},\sigma}(r)\) over a primitive unit cell (\(\sigma = \pm\) give the same matrix elements), and \(\theta_k\) is the polar angle of \(r_k\).

The magnetic moment of a HH is inverted with respect to that for an electron. This results in a change of sign in Eqs. (2)-4 and leads to the minus sign in Eq. 7 and of the values in columns (i) and (ii) of Table I.

D. Non-Ising corrections

There will be small corrections to the form of the effective Hamiltonian given in Eq. 11. Evaluating off-diagonal matrix elements of \(H\) and of \(\Delta_{\text{HH}}\) with the approximate Bloch amplitudes \(|\phi; u_{\text{HH},\sigma}\rangle\) leads to minimal non-Ising corrections, whose associated coupling strengths \(A_{\text{HH}}^k\) we find to be small: \(A_{\text{HH}}^k < 0.06 A_k^l\). Higher-order virtual transitions between the \(m_f = \pm 3/2\) states via the LH sub-band are suppressed by \(\sim A_k^b/\Delta_{\text{HH}} \ll 1\). Hybridization with other bands can also lead to non-Ising corrections. For unstrained quantum dots, we find that these corrections are small: typically on the order of 1% of the values given in Table I (see also Appendix A). Strain can lead to considerably stronger band mixing and, hence, to significantly larger non-Ising corrections to Eq. 11.

III. Spin decoherence

Now that the effective Hamiltonian (Eq. 11) has been established, we can analyze the dephasing of a HH pseudospin in the presence of a random nuclear environment. In an applied magnetic field, pseudospin dynamics of the HH are described by the Hamiltonian

\[
H = (b_x + h_x) s_x + b_y s_y,
\]

where \(h_z = \sum_k A_k^h r_k^z\) is the nuclear field operator, \(b_x = g_x \mu_B B_z\) is the Zeeman splitting due to a magnetic field \(B_z\) along the growth direction, and \(b_y = g_y \mu_B B_x\) is the Zeeman splitting due to an applied magnetic field \(B_x\) in the plane of the quantum dot. \(g_x\) and \(g_y\) are the components of the HH g-tensor along the growth direction and in the plane of the quantum dot, respectively (we assume the in-plane g-tensor to be isotropic).

If no special effort is made to control the nuclear field,
the field value will be Gaussian-distributed in the limit of a large number of nuclear spins. The variance for a random nuclear-spin distribution is (see Appendix D)

$$\langle h_z^2 \rangle = \sigma^2 \simeq \frac{1}{4N} \sum_j v_j \rho_j (\rho_j + 1) (A_{h}^j)^2,$$  \hfill (9)

where $N = \pi^2 a_z/v_0$ is the number of nuclei within the quantum dot. The nuclear-field fluctuation $\sigma$ therefore inherits a magnetic-field dependence from $l$ (see Eq. (9)). A finite nuclear-field variance will result in a random distribution of precession frequencies experienced by the hole pseudospin, inducing pure dephasing (decay of the components of hole pseudospin transverse to B).

First, we consider the case $b_\parallel = 0$. For a hole pseudospin initially oriented along the $x$ direction, we find a Gaussian decay (see Fig. 1 (a)) of the transverse pseudospin in the rotating frame $\langle \hat{s}_+ \rangle_t = \exp(-ib_\perp t) \left( \langle s_x \rangle_t + i \langle s_y \rangle_t \right)$:

$$\langle \hat{s}_+ \rangle_t = \frac{1}{2} \exp \left( -\frac{t^2}{2\tau_{\perp}^2} \right), \quad \tau_{\perp} = \frac{1}{\sigma}. \hfill (10)$$

This is the same Gaussian decay that occurs for electrons. Here, since the magnetic field is taken to be out-of-plane, we must account of the diamagnetic “squeezing” of the wavefunction. This squeezing affects the number $N$ of nuclear spins within the dot and hence, the finite-size fluctuation $\sigma$. The coherence time $\tau_L(B_z) = 1/\sigma(B_z) = \tau_{\perpendicular}(0) \left[ 1 + (B_z/B_0)^2 \right]^{-1/4}$ then decreases for large $B_z$ (see Fig. 1 (b)). This undesirable effect can be avoided for confined electron spins by generating a large Zeeman splitting through an in-plane (rather than out-of-plane) magnetic field. This option may not be available for a HH where, typically, $g_\| \ll g_\perp$.

The situation changes drastically for an in-plane magnetic field ($b_\perp = 0$). In this case, since the hyperfine fluctuations are purely transverse to the applied field direction, the decay is given by a slow power law at long times (see Fig. 1 (c)) and the relevant dephasing time increases as a function of the applied magnetic field (see Fig. 1 (d)). In the limit $b_\parallel \gg \sigma$ and for a HH pseudospin initially prepared along the $z$-direction, we find

$$\langle \hat{s}_z \rangle_t \simeq \cos \frac{b_\parallel t + \frac{1}{2} \arctan(t/\tau_L)}{2[1 + (t/\tau_L)^2]^{1/4}}, \quad \tau_L = \frac{b_\parallel}{\sigma^2}. \hfill (11)$$

The derivation of Eq. (11) is directly analogous to that for the decay of driven Rabi oscillations in Ref. 34.

### IV. ESTIMATES OF THE COUPLING STRENGTHS

To estimate the size of $A_h$, we need an explicit expression for the HH $k = 0$ Bloch amplitudes. We approximate $u_{HH0}\sigma(r)$ within a Wigner-Seitz cell centered halfway along the Ga-As bond by a linear combination of atomic orbitals, following Ref. 36:

$$u_{HH0}\sigma(r)\bigg|_{r \in WS} = N_{\alpha_e} \left( \alpha_e \Psi_{6s}^{Ga}(r + d/2) + \sqrt{1 - \alpha_e^2} \Psi_{4s}^{As}(r - d/2) \right). \hfill (12)$$

Here, $d = \frac{a}{2}(1,1,1)$ is the Ga-As bond vector, $\alpha$ is the lattice constant, $\alpha_e$ describes the relative electron sharing at the Ga and As sites in the HH sub-band, and $N_{\alpha_e}$ is a normalization constant, chosen to enforce $\int_{WS} d^3r |u_{HH0}\sigma(r)|^2 = 2$, where the integration is performed over the Wigner-Seitz cell defined above. To simplify numerical integration, we replace the Wigner-Seitz cell by a sphere centered halfway along the Ga-As bond, with radius given by half the Ga-Ga nearest-neighbor distance. We find the electron sharing in the CB from the densities given in Ref. 35 to be $\alpha_e^2 \simeq 1/2$ (see Appendix D) and assume the same ($\alpha_e^2 = 1/2$) for Eq. (12). Using $Z_{off}$ for free atoms, we evaluate Eq. (7) with the ansatz, Eq. (12), by numerical integration, giving the values shown in Table I column (i). We check the validity of this procedure by writing the CB Bloch amplitudes as in Eq. (12), replacing the $4p$-eigenfunctions by $4s$-eigenfunctions. Evaluating the coupling constants for the CB ($A_e^j$) from $h_z^j$ gives the numbers in column (ii). The accepted values of $A_e^j$ from Ref. 35 are shown in column (iv) for comparison. Our method produces $A_e^j$ within a factor of two of the accepted values. Our procedure, which relies on free-atom orbitals, most likely under-estimates the electron density near the atomic sites, which should be enhanced in a solid due to confinement. Assuming the relative change in density going from a free atom to a solid is the same for the CB and HH band, we rescale the results in column (i) by the ratio of the values in columns (iv) and (iii), giving column (ii). Due to the approximations involved, we expect the values in columns (i) and (ii) only to be valid to within a factor of two or three.

| $\alpha$ | $A_h^\alpha$ (\text{\textmu eV}) | $A_e^\alpha$ (\text{\textmu eV}) |
|---|---|---|
| $^{69}\text{Ga}$ | -7.1 | -13 |
| $^{71}\text{Ga}$ | -9.0 | -17 |
| $^{75}\text{As}$ | -8.2 | -12 |

TABLE I: Estimates of the coupling strengths for a HH ($A_h^\alpha$) and a CB electron ($A_e^\alpha$) for the three isotopes in GaAs. Columns (i) and (iii) show values obtained from a linear combination of hydrogenic eigenfunctions, using free-atom values of $Z_{off}$ calculated in Ref. 34. Column (iv) gives the accepted values of $A_e^\alpha$ from Ref. 35. Column (ii) shows the rescaled values from column (i) (see text). In the last row we give the average coupling constants weighted by the natural isotopic abundances: $\nu_{69}\text{Ga} = 0.3$, $\nu_{71}\text{Ga} = 0.2$, $\nu_{75}\text{As} = 0.5$. 

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V. CONCLUSIONS

We have shown that the interaction of a quantum-dot-confined heavy hole with nuclear spins is stronger than previously anticipated. We have estimated the associated coupling strength to be on the order of 10μeV in GaAs – only one order of magnitude less than the hyperfine coupling for electrons. However, the interaction turns out to be Ising-like which has profound consequences for hole-spin decoherence. Since no flip-flop terms occur in the effective Hamiltonian (Eq. (1)), the main source of decoherence is given by the broad frequency distribution of the nuclear spins. Recent theoretical and experimental studies have shown that state-narrowing techniques are capable of strongly suppressing this source of decoherence, which makes the heavy hole an attractive spin-qubit candidate.

Very recently, experimental results on hole-spin relaxation in self-assembled quantum dots have been released. Gerardot et al. report an extremely weak coupling of HH spin states, which is explained by our theory to be a direct consequence of the Ising-like nuclear-spin interaction (negligible flip-flop terms). Eble et al., in contrast, find very short hole-spin relaxation times on the order of 15 nanoseconds. This is due to the strong strain present in the particular dots used in this experiment, resulting in a considerable HH-LH mixing and a highly non-Ising interaction (large flip-flop terms).

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APPENDIX A: HEAVY-HOLE STATES

In this section we give details on our derivation of an approximate basis of heavy-hole (HH) eigenstates in a quantum dot. We will approximate the ground-state quantum-dot envelope function in the HH sub-band by

\[ \phi(r) = \phi_z(z) \phi_\rho(\rho), \]

\[ \phi_\rho(\rho) = \frac{1}{\sqrt{\pi l}} \exp \left( -\frac{\rho^2}{2l^2} \right), \]

\[ \phi_z(z) = \sqrt{\frac{2}{a_z}} \sin \left( \frac{\pi z}{a_z} \right), \quad z = [0 \ldots a_z], \]

where \( a_z \) is the width of the confinement potential along the growth direction (for definition of the other symbols see Eq. (2)). We will then estimate the size of the splitting \( \Delta_{HH} \) between the HH and the light-hole (LH) band and the degree of hybridization with the conduction band (CB), LH and split-off (SO) sub-bands.

We start from the 8 × 8 Kane Hamiltonian given in Ref. [37] for bulk zinc-blende-type crystals, which is written in terms of the exact eigenstates (near \( k = 0 \)) of an electron in the CB, HH, LH and SO band, usually denoted by \( |1/2; \pm 1/2\rangle_v, |3/2; \pm 3/2\rangle_v, |3/2; \pm 1/2\rangle_v, \) and \( |1/2; \pm 1/2\rangle_v \), respectively. We neglect terms that are more than two orders of magnitude smaller than the fundamental band-gap energy \( E_{g,40} \) and perform the quasi-two-dimensional limit by assuming that a confinement potential has been applied along the growth direction. If the confinement potential is sufficiently strong (i.e., if the quantum well is sufficiently narrow), the energy-level spacing will be large and the electron will be in the ground state at low temperatures. Any operator acting on the \( z \)-component of the electron envelope function can then be replaced by its expectation value with respect to the \( z \)-component of the ground-state envelope function. For the Kane Hamiltonian this means that we can replace powers of the \( z \)-component of the electron envelope function along the growth direction, the ground state is given by Eq. (A3). Calculating the expectation value of \( k_z^2 \) and \( k_z^4 \) with respect to the ground state, we find \( \langle k_z \rangle = 0 \) and \( \langle k_z^2 \rangle = \pi^2/(a_z^2) \). This allows us to write the Kane Hamiltonian in the following form:

\[ H_K = \begin{pmatrix} H_{CB} & V_1 & V_2 & V_3 \\ V_1^\dagger & H_{HH} & V_4 & V_5 \\ V_2^\dagger & V_4^\dagger & H_{LH} & V_6 \\ V_3^\dagger & V_5^\dagger & V_6^\dagger & H_{SO} \end{pmatrix}, \]

where

\[ H_{CB} = \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}, \quad H_{HH} = \begin{pmatrix} B & 0 \\ 0 & B \end{pmatrix}, \]

\[ H_{LH} = \begin{pmatrix} C & 0 \\ 0 & C \end{pmatrix}, \quad H_{SO} = \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}, \]

\[ V_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} -E & 0 \\ 0 & E^* \end{pmatrix}, \quad V_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & E^* \\ -E & 0 \end{pmatrix}, \]

\[ V_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & E^* \\ -E & 0 \end{pmatrix}, \quad V_4 = \sqrt{3} \begin{pmatrix} 0 & F \\ -F & 0 \end{pmatrix}, \]

\[ V_5 = \sqrt{3} \begin{pmatrix} F & 0 \\ 0 & F \end{pmatrix}, \quad V_6 = \frac{1}{\sqrt{2}} \begin{pmatrix} -G & 0 \\ 0 & G \end{pmatrix}, \]

and

\[ A = E_y + \hbar^2 (k_x^2 + k_y^2 + \langle k_z^2 \rangle)/2m', \]

\[ B = -\epsilon (\gamma_1' + \gamma_2' (k_x^2 + k_y^2) + (\gamma_1' - 2\gamma_2') \langle k_z^2 \rangle), \]

\[ C = -\epsilon (\gamma_1' - \gamma_2' (k_x^2 + k_y^2) + (\gamma_1' + 2\gamma_2') \langle k_z^2 \rangle), \]

\[ D = -\epsilon \gamma_1' (k_x^2 + k_y^2 + \langle k_z^2 \rangle) - \Delta_{SO}, \]

\[ E = Pk_z, \]

\[ F = \epsilon (\gamma_2' (k_x^2 - k_z^2) - 2i\gamma_1' k_y k_z), \]

\[ G = \epsilon \gamma_2' (k_x^2 + k_y^2 - 2\langle k_z^2 \rangle). \]

Here, \( \epsilon = \hbar^2/2m_0 \) and \( m_0 \) is the free-electron mass, whereas \( m' \) is the effective mass of a CB electron. Fur-
thermore, \( k_\pm = k_x \pm ik_y \), \( \gamma' \) denote the Luttinger parameters, \( P \) is the inter-band momentum, and \( \Delta_{SO} \) is the spin-orbit gap between the LH and the SO bands. Experimental values for these parameters can be found in Table I.

We assume a circular-symmetric parabolic confinement potential with frequency \( \omega_0 \) in the \( xy \)-plane defining a quantum dot. Including a magnetic field along the growth direction, the ground state is approximately described by the Gaussian given in Eq. (A2). The envelope function of the quantum dot is then the product of the in-plane and out-of-plane components, as given in Eq. (A1).

In the quasi-two-dimensional limit, a gap

\[
\Delta_{\text{LH}} = (B-C) = -\frac{k^2 \gamma_2}{m_0} \left( \langle k_x^2 \rangle + \langle k_y^2 \rangle - 2 \langle k_z^2 \rangle \right) \quad (A5)
\]

develops between the HH and LH sub-bands, lifting the HH-LH degeneracy. Here, \( \langle \cdots \rangle \) denotes the expectation value with respect to \( |A\rangle \). The in-plane level spacing scales like \( \sim 1/l^2 \), where \( l \) is the dot Bohr radius. The in-plane level spacing is much smaller than the level spacing along the growth direction since, for typical dots, \( a_z^2 \ll l^2 \). Neglecting \( \langle k_z^2 \rangle \) and \( \langle k_y^2 \rangle \) compared to \( \langle k_x^2 \rangle \) in Eq. (A5) and inserting \( \langle k_x^2 \rangle = \pi^2/\sigma_z^2 \) for a square-well potential, we estimate

\[
\Delta_{\text{LH}} \simeq \frac{2\pi^2 \gamma_2}{\sigma_z^2 m_0} \approx 100 \text{ meV} \quad (A6)
\]

for \( a_z \approx 5 \text{ nm} \), using \( \gamma_2 \approx 2.06 \) for GaAs (see Table I). The HH-LH splitting is thus much larger than the typical energy scale associated with the hyperfine interaction (\( A_e \approx 90 \mu eV \) for CB electrons in GaAs).

To derive the approximate electron eigenfunctions in the HH sub-band of the quantum well, we start from the Kane Hamiltonian \( \mathcal{H}_K \). We use quasi-degenerate perturbation theory up to first order in \( 1/E \) (where \( E \) stands for \( E_g, \Delta_{\text{LH}}, \) or \( \Delta_{\text{LH}} + \Delta_{SO} \)), taking \( H_{HH} \) as the unperturbed Hamiltonian. This leads to a band-hybridized state of the form

\[
|\Psi_{\text{HH,hyb}}\rangle = N_{\sigma} \sum_n \lambda_\sigma^+ |\phi_{\sigma u}; n0\rangle \quad (A7)
\]

Here, \( \sigma = \pm, \langle r|\phi_{\sigma u}; n0\rangle = \sqrt{v} \phi_{\sigma u}(r) u_{n0}\langle r \rangle \) is the product of envelope function and \( k = 0 \) Bloch amplitude in band \( n \) (CB, HH, LH or SO), the prefactors \( \lambda_\sigma^+ \) describe the degree of band hybridization, and \( N_{\sigma} \) enforces proper normalization.

In first order quasi-degenerate perturbation theory, the hybridization with the CB and the LH and SO sub-bands is described by the interaction terms \( V_1, V_4 \), and \( V_5 \) in Eq. (A4), respectively. We estimate the degree of hybridization by applying these operators to a two-spinor containing the in-plane ground-state envelope function \( \langle A \rangle \) of the HH sub-band. For the hybridization with the conduction band, we find (for \( B = 0 \))

\[
\frac{1}{E_g} V_1 \left( \phi_+^1 (\rho) \phi^-_1 (\rho) \right) = \left( \lambda^+_{CB} \phi_{CB+}(\rho) / \lambda_{CB} \phi_{CB-}(\rho) \right) \quad (A8)
\]

where

\[
\phi_{CB\rho}(\rho) = i \sqrt{2} (\psi_{10}(\rho) \pm i \psi_{01}(\rho)) \quad (A9)
\]

Here, \( \psi_{nm}(\rho) = \psi_n(x) \psi_m(y) \) and \( \psi_n(x) \) is the \( n \)-th harmonic-oscillator eigenstate. The envelope function of the admixed CB state is a superposition of excited harmonic-oscillator eigenfunctions. The prefactor

\[
\lambda_{CB}^+ = \pm \frac{P}{\sqrt{2E_g}} \quad (A10)
\]

determines the degree of \( sp \)-hybridization. Using values from Table I and assuming a quantum dot with dot Bohr radius \( l_0 \approx 30 \text{ nm} \) (\( B = 0 \)), we estimate \( \lambda_{CB}^+ \approx 10^{-2} \). Similarly, we estimate \( \lambda_{HH}^+ \approx 3 \times 10^{-3} \), assuming a dot height \( a_z \approx 5 \text{ nm} \). The admixture of CB, LH and SO states to the HH state is thus on the order of \( 1\% \) and has therefore been neglected in our considerations.

We emphasize that \( sp \)-hybridization will lead to a coupling of the HH to the nuclear spins via the Fermi contact interaction. Since the Fermi contact interaction is of Heisenberg-type, \( sp \)-hybridization will directly lead to non-Ising corrections to the effective Hamiltonian given in Eq. (1). The size of these corrections is determined by the degree of \( sp \)-hybridization which is on the order of \( 1\% \) (see above).

### APPENDIX B: ESTIMATE OF THE FERMI CONTACT INTERACTION

In Eq. (12), we have approximated the HH \( \mathbf{k} = 0 \) Bloch amplitudes within a Wigner-Seitz cell by a linear combination of atomic orbitals. Similarly, we approximate the \( \mathbf{k} = 0 \) Bloch amplitude in the CB by

\[
u_{CB\sigma}(r)|_{r \in WS} = N_{\sigma} \left( \alpha_{e} \Psi_{4\gamma_0}(r + \mathbf{d}/2) - \sqrt{1 - \alpha_{e}^2} \Psi_{4\gamma_0}(r - \mathbf{d}/2) \right), \quad (B1)
\]

independent of \( \sigma \). Here, \( \Psi_{4\gamma_0}(r) = R_{4\gamma}(r) Y_{4\gamma}^0(\theta, \phi) \), \( \alpha_{e} \) describes the relative electron sharing between the Ga and As atom in the Wigner-Seitz cell chosen to be centered halfway along the Ga-As bond, and \( N_{\sigma} \) normalizes the Bloch amplitude to two atoms in a primitive unit cell. The radial wavefunction depends implicitly on the effective nuclear charges \( Z_{eff}(\kappa, 4\gamma) \), where \( \kappa = \text{Ga, As} \).

We will estimate the relative electron sharing in the CB by calculating the electron densities at the sites of the

| Parameter | Value |
|-----------|-------|
| \( P \) (eV) | 10.5 \* |
| \( E_g \) (eV) | 1.52 \* |
| \( \Delta_{SO} \) (eV) | 0.34 \* |

\* taken from Ref. 1, 2

\( \gamma_2 \approx 2.06 \text{ for GaAs} \) (see Table II).
nuclei from Eq. (B1) and comparing to accepted values taken from Ref. 33. We will then estimate the Fermi contact interaction of a CB electron using free-atm effective nuclear charges taken from Ref. 31 (\(Z_{\text{eff}}(\text{Ga, 4s}) \approx 7.1\), \(Z_{\text{eff}}(\text{Ga, 4p}) \approx 6.2\), \(Z_{\text{eff}}(\text{As, 4s}) \approx 8.9\), and \(Z_{\text{eff}}(\text{As, 4p}) \approx 7.4\)) and normalizing the Bloch amplitude over a Wigner-Seitz cell.

We approximate the electron densities at the Ga and As sites within a primitive unit cell from Eq. (B1):

\[
d_{\text{Ga}} = |u_{\text{CBGa}}(-\mathbf{d}/2)|^2 \approx \alpha_{\text{Ga}}^2 |\Psi_{400}^{\text{Ga}}(0)|^2, \quad (\text{B2})
\]

\[
d_{\text{As}} = |u_{\text{CBAs}}(+\mathbf{d}/2)|^2 \approx \alpha_{\text{As}}^2 |\Psi_{400}^{\text{As}}(0)|^2. \quad (\text{B3})
\]

We estimate the corrections to the right-hand sides to be on the order of 1% due to overlap terms. We take the ratio \(d_{\text{Ga}}/d_{\text{As}}\) and equate this with the ratio of the values from Ref. 33, \(d_{\text{Ga}}' = 5.8 \times 10^{-31} \text{ m}^{-3}\) and \(d_{\text{As}}' = 9.8 \times 10^{-31} \text{ m}^{-3}\). This allows us to write \(\alpha_c\) as a function of the two effective nuclear charges:

\[
\alpha_c = \left[ 1 + \frac{d_{\text{As}}'}{d_{\text{Ga}}'} \left( \frac{Z_{\text{eff}}(\text{Ga, 4s})}{Z_{\text{eff}}(\text{As, 4s})} \right)^3 \right]^{-1/2}. \quad (\text{B4})
\]

Recalling that \(N_{\alpha_c}\) normalizes the Bloch amplitude to two atoms over a Wigner-Seitz cell, we write

\[
N_{\alpha_c} = \left[ \frac{1}{2} \int_{WS} d^3r \left( \alpha_c \Psi_{400}^{\text{Ga}}(r + \mathbf{d}/2) - \sqrt{1 - \alpha_c^2} \Psi_{400}^{\text{As}}(r - \mathbf{d}/2) \right)^2 \right]^{-1/2}. \quad (\text{B5})
\]

For all numerical integrations, we approximate the Wigner-Seitz cell by a sphere centered halfway along the Ga-As bond with radius equal to half the Ga-Ga nearest-neighbor distance. Inserting (B4) and (B5) into (B2) and (B3), we solve the two coupled equations

\[
d_{\text{Ga}}(Z_{\text{eff}}(\text{Ga}, Z_{\text{eff}}(\text{As})) - d_{\text{Ga}}') = 0, \quad (\text{B6})
\]

\[
d_{\text{As}}(Z_{\text{eff}}(\text{Ga}, Z_{\text{eff}}(\text{As})) - d_{\text{As}}') = 0, \quad (\text{B7})
\]

for the two effective nuclear charges. This yields \(Z_{\text{eff}}(\text{Ga}) \approx 9.8\) and \(Z_{\text{eff}}(\text{As}) \approx 11.0\). Inserting these values back into Eq. (B4), we estimate the electron sharing within the primitive unit cell to be

\[
\alpha_c^2 \approx 0.46. \quad (\text{B8})
\]

For comparison, inserting free-atm effective nuclear charges into Eq. (B1) yields a similar value: \(\alpha_c^2 \approx 0.54\).

Now we estimate the Fermi contact interaction of a CB electron starting from the free-atm effective nuclear charges \(Z_{\text{eff}}(\kappa, 4s)\) obtained from Ref. 31. We use \(\alpha_c \approx 1/\sqrt{2}\) and normalize the \(\mathbf{k} = 0\) Bloch amplitude to two atoms over a Wigner-Seitz cell, following Eq. (B5). From the normalized Bloch amplitudes we estimate the Fermi contact hyperfine interaction by evaluating

\[
A_j = \frac{2\mu_0}{3} \gamma_s \gamma_j |u_{\text{CB}}(\mathbf{R}_j)|^2. \quad (\text{B9})
\]

Here, \(\mathbf{R}_j = \pm\mathbf{d}/2\) for Ga and As, respectively (\(j\) indexes the nuclear isotope). Evaluating for the isotopes in GaAs, this gives the values shown in column (iii) of Table I.

Replacing the Wigner-Seitz cell by a sphere with radius \(R_s\) equal to half the Ga-Ga nearest-neighbor distance in our numerical integrations overestimates the expectation value of \[\tau_k^2(1 + d/r_k)^{-1}\] in Eq. (4). To estimate the error, we perform an integration over a sphere with radius \(R' = (R_s + R_{\text{max}})/2\), where \(R_{\text{max}}\) denotes the radius of the smallest sphere that fully contains the Wigner-Seitz cell. From this, we estimate the relative error to be less than 30%.

**APPENDIX C: ESTIMATE OF THE LONG-RANGED INTERACTIONS**

In this section, we estimate the corrections to the HH coupling strength in Eq. (7) due to long-ranged dipole-dipole interactions and long-ranged \(\mathbf{L} \cdot \mathbf{I}\) interactions. To this end, we consider a single nucleus interacting with a HH that is delocalized over the lattice sites in the quantum dot. We start from the Hamiltonians given in Eqs. (3) and (4). We define effective radii \(a_{\text{eff}}(\kappa, 4p) = a_0/Z_{\text{eff}}(\kappa, 4p)\), where \(a_0 \approx 5.3 \times 10^{-11} \text{ m}\) is the Bohr radius. The effective radii define an approximate length scale for the spread of the site-localized functions \(\Psi_{\text{LD}(\mathbf{r})}\) and are much smaller than the GaAs lattice constant \(a_L \approx 5.7 \times 10^{-10} \text{ m}\). The nuclei thus effectively ‘see’ sharp-peak electron densities centered around the more distant lattice sites. We choose the nucleus to be at site \(\mathbf{R}_k\) and estimate the interaction with the electron density at more distant atomic sites by approximating the electron densities by \(\delta\)-functions. Adding up contributions from \(h^2\) and \(h^4\), we arrive at an effective Hamiltonian describing the long-ranged interactions:

\[
H_{\text{lr}} = A_k^{\text{ii}} \delta_{\mathbf{R}_k} \rho, \quad (\text{C1})
\]

where \(A_k^{\text{ii}} = \sum_{l \neq k} A_{kl}^{\text{ii}}\) is the associated coupling strength and \(A_{kl}^{\text{ii}} = \psi_n(\phi(\mathbf{R}_k))|2 \int d^3r_\ell \delta(r_k - r_\ell)(h^2 + h^2)|\) describes the coupling of the electron density at site \(\mathbf{R}_k\) to the nucleus at site \(\mathbf{R}_k\) (\(A_{kl}^{\text{ii}} = h^2\)). In order to estimate the size of the long-ranged interactions relative to the on-site interactions, we take into account nearest-neighbor couplings for the long-ranged part, i.e., we replace \(\sum_{l \neq k} \sum_{l = \text{n.n.}} \) \(\sum_{l = \text{n.n.}}\). The interaction with electron density located around more distant nuclei is suppressed by \(\sim 1/R_k^2\). Assuming that the quantum-dot envelope function varies slowly over the nearest-neighbor distance \((\phi(\mathbf{R}_k) \approx \phi(\mathbf{R}_k))\) for \(l\) nearest neighbor of \(k\), we estimate the ratio of long-ranged and on-site interactions (Table I, column (i)) to be

\[
A_k^{\text{ii}} / A_k \approx 7 \times \times 10^{-3}, \quad (\text{C1})
\]

on the order of 1%, where \(A_k^{\text{ii}} = \psi_n(\phi(\mathbf{R}_k))|2 \int d^3r_\ell \delta(r_k - r_\ell)(h^2 + h^4)|\) describes the electron g-factor can deviate from the free-electron g-factor due to spin-orbit interaction. According to Ref. 39, this renormalization
is negligible for the on-site interaction, but could become relevant for the long-ranged interaction. However, for the estimate in Eq. (C1), we have taken the free-electron g-factor.

APPENDIX D: VARIANCE OF THE NUCLEAR FIELD

Here we calculate the nuclear-field variance for a HH interacting with nuclei in a quantum dot. In particular, we evaluate

\[ \sigma^2 = \langle h_z^2 \rangle, \quad (D1) \]

where \( \langle \cdots \rangle = \text{Tr} \{ \rho \cdots \} \) indicates the expectation value with respect to the infinite-temperature thermal equilibrium density matrix \( \rho_I \) and we recall \( h_z = \sum_k A_k^h I_k^z \). For an uncorrelated and unpolarized nuclear state, we have

\[ \langle I_k^z I_{k'}^z \rangle = \langle I_k^z \rangle \langle I_{k'}^z \rangle = 0, \quad k \neq k', \]

which gives

\[ \sigma^2 = \sum_k (A_k^h)^2 \langle \langle I_k^z \rangle^2 \rangle. \quad (D2) \]

Using \( \langle \langle I_k^z \rangle^2 \rangle = I^z (I^z + 1) / 3 \) for an infinite-temperature state, \( A_k^h = A_k^h v_0 |\phi(R_k)|^2 \), and assuming that the nuclear isotopic species with abundances \( \nu_j \) are distributed uniformly throughout the dot gives

\[ \sigma^2 = \frac{1}{3} I_0 \sum_j \nu_j I^z (I^z + 1) (A_j^h)^2, \quad (D3) \]

where

\[ I_0 = v_0^2 \sum_k |\phi(R_k)|^4. \quad (D4) \]

Assuming that the envelope function \( \phi(r) \) varies slowly on the scale of the lattice, we replace the sum in Eq. (D4) by an integral:

\[ v_0 \sum_k |\phi(R_k)|^4 \rightarrow \int d^3 r |\phi(r)|^4. \quad (D5) \]

Inserting the envelope functions (A2) and (A3) for a quantum dot with height \( a_z \) and radius \( l \) and evaluating the integral in Eq. (D5), we find

\[ I_0 = \frac{3}{4} \frac{1}{N}. \quad (D6) \]

Here, \( N \) is the number of nuclear spins within the quantum dot, given explicitly by

\[ N = \frac{\pi l^2 a_z}{v_0}. \quad (D7) \]

Inserting Eq. (D6) into Eq. (D3) directly gives Eq. (9).

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40 In Winkler’s notation \( C, B_{7\nu}, \text{ and } B_{8\nu}^\pm \), these are the terms proportional to \( C_k \), \( B_{7\nu} \), and \( B_{8\nu}^\pm \). These terms will not lead to considerable corrections for our purposes. However, the terms \( C_{k\pm} \) could become relevant when considering higher-order effects in the spin-orbit interaction, such as the cubic Dresselhaus terms which were derived in Ref. 17.