Supporting Information:
Heavy-Hole States in Germanium Hut Wires

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Finite element simulations of the strain in a HW

The two images in Figure 1 represent COMSOL simulations of the out-of-plane (left) and the in-plane (right) strain distribution of a capped HW. For our theoretical model we have extracted an out-of-plane value of 2 and an in-plane value of -3.3 percent.

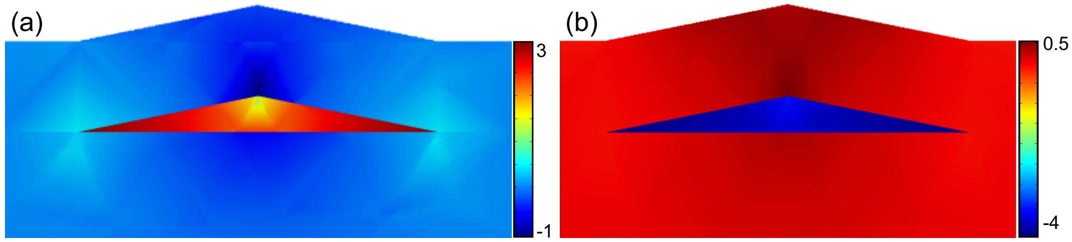

Figure 1: COMSOL simulations of the out-of-plane (a) and the in-plane strain distribution (b) in a capped HW. The color scale represents the percentage of strain with positive (negative) values meaning tensile (compressive) strain.

Matrix representation of spin operators

We use the following matrix representation[1] for the operators J_ν. The basis states are $|3/2\rangle$, $|1/2\rangle$, $|-1/2\rangle$, and $|-3/2\rangle$.

$$J_x = \begin{pmatrix} 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & 0 & 1 & 0 \\ 0 & 1 & 0 & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 \end{pmatrix}, \quad J_y = \begin{pmatrix} 0 & -i\frac{\sqrt{3}}{2} & 0 & 0 \\ i\frac{\sqrt{3}}{2} & 0 & -i & 0 \\ 0 & i & 0 & -i\frac{\sqrt{3}}{2} \\ 0 & 0 & i\frac{\sqrt{3}}{2} & 0 \end{pmatrix}, \quad J_z = \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}. \tag{1}$$

In the derivation of the pure-HH Hamiltonian [Eq. (34)], we consider the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2}$$

where $|3/2\rangle$ and $|-3/2\rangle$ are the basis states.

Calculation with electric fields

It is well possible that an electric field E_z along the out-of-plane axis was present in the experiment. When the direct coupling $-eE_z z$ and the standard Rashba spin-orbit coupling $\alpha E_z(k_x J_y - k_y J_x)$, with $\alpha = -0.4$ nm$^2 e$,[1,2] are added to the Hamiltonian H [Eq. (1) of the main text], our finding that the low-energy states correspond to HH states remains unaffected, even for strong E_z around 100 V/μm. Due to symmetries in our setup, we believe that electric fields E_y along y were very small. Nevertheless, we find numerically that the HH character of the eigenstates is preserved even when the direct and the standard Rashba coupling that are caused by nonzero E_y are included in the model. We note that additional corrections besides the standard Rashba spin-orbit interaction arise for hole states in the presence of an electric field,[1] but these terms are all small and will not change our result that the low-energy states are of HH type.

Couplings $C_\pm$

Here we explain the calculation of the matrix elements $C_\pm$ that are presented in Eq. (4) of the main text. When the magnetic field is applied along the z axis, the Hamiltonian is

$$\begin{aligned} H &= \frac{\hbar^2}{2m}\left[\left(\gamma_1 + \frac{5\gamma_2}{2}\right)k^2 - 2\gamma_2 \sum_\nu k_\nu^2 J_\nu^2 - 4\gamma_3\left(\{k_x, k_y\}\{J_x, J_y\} + \text{c.p.}\right)\right] \\ &\quad +2\mu_B B_z\left(\kappa J_z + q J_z^3\right) + b\sum_\nu \epsilon_{\nu\nu} J_\nu^2 + V(y,z) \end{aligned} \tag{3}$$

and the vector potential is $\boldsymbol{A} = (-B_z y, 0, 0)$. Consequently,

$$\{k_y, k_z\} = -\partial_y \partial_z, \tag{4}$$

$$\{k_x, k_z\} = -\partial_x \partial_z + i\frac{e}{\hbar}B_z y \partial_z, \tag{5}$$

$$\{k_x, k_y\} = -\partial_x \partial_y + i\frac{e}{\hbar}B_z y \partial_y + i\frac{e}{2\hbar}B_z, \tag{6}$$

$$k_x^2 = -\partial_x^2 + 2i\frac{e}{\hbar}B_z y \partial_x + \frac{e^2}{\hbar^2}B_z^2 y^2, \tag{7}$$

and $k_y^2 = -\partial_y^2$, $k_z^2 = -\partial_z^2$. Using the matrices for the spin operators J_ν listed in Eq. (1), one finds

$$\begin{aligned} \langle \pm 3/2| \{J_y, J_z\} |\pm 1/2\rangle &= -i\frac{\sqrt{3}}{2}, & (8)\\ \langle \pm 3/2| \{J_x, J_z\} |\pm 1/2\rangle &= \pm\frac{\sqrt{3}}{2}, & (9) \end{aligned}$$

whereas

$$\langle \pm 3/2| Q |\pm 1/2\rangle = 0 \tag{10}$$

when the operator Q is $\{J_x, J_y\}$, J_x^2, J_y^2, J_z^2, J_z, or J_z^3. Therefore,

$$\begin{aligned} C_\pm &= \langle \pm 3/2, 1, 1, 0| H |\pm 1/2, 2, 2, 0\rangle \\ &= i\sqrt{3}\frac{\gamma_3\hbar^2}{m} \langle \varphi_{1,1,0}| \{k_y, k_z\} |\varphi_{2,2,0}\rangle \mp \sqrt{3}\frac{\gamma_3\hbar^2}{m} \langle \varphi_{1,1,0}| \{k_x, k_z\} |\varphi_{2,2,0}\rangle, \qquad (11) \end{aligned}$$

where the wave functions [see Eq. (3) of the main text] of the basis states are

$$\begin{aligned} \varphi_{1,1,0} &= \frac{2}{\sqrt{L_z L_y}} \sin\left[\pi\left(\frac{z}{L_z} + \frac{1}{2}\right)\right] \sin\left[\pi\left(\frac{y}{L_y} + \frac{1}{2}\right)\right], & (12)\\ \varphi_{2,2,0} &= \frac{2}{\sqrt{L_z L_y}} \sin\left[2\pi\left(\frac{z}{L_z} + \frac{1}{2}\right)\right] \sin\left[2\pi\left(\frac{y}{L_y} + \frac{1}{2}\right)\right] & (13) \end{aligned}$$

inside the HW ($|z| < L_z/2$, $|y| < L_y/2$) and $\varphi_{1,1,0} = 0 = \varphi_{2,2,0}$ outside. We note that $\langle \varphi_{1,1,\tilde{k}_x}| \partial_x\partial_z |\varphi_{2,2,\tilde{k}_x}\rangle$ vanishes for arbitrary $\tilde{k}_x$ after integration over the y axis due to the orthogonality of the basis functions for the y direction. Thus, using Eqs. (4) and (5) in Eq. (11) yields

$$C_\pm = -i\sqrt{3}\frac{\gamma_3\hbar^2}{m} \langle \varphi_{1,1,0}| \partial_y\partial_z |\varphi_{2,2,0}\rangle \mp i\sqrt{3}\frac{\gamma_3 e\hbar}{m} B_z \langle \varphi_{1,1,0}| y\partial_z |\varphi_{2,2,0}\rangle. \tag{14}$$

With the integrals (analogous for z)

$$\int_{-L_y/2}^{L_y/2} dy \sin\left[\pi\left(\frac{y}{L_y}+\frac{1}{2}\right)\right]\frac{2\pi}{L_y}\cos\left[2\pi\left(\frac{y}{L_y}+\frac{1}{2}\right)\right] = -\frac{4}{3}, \tag{15}$$

$$\int_{-L_y/2}^{L_y/2} dy \sin\left[\pi\left(\frac{y}{L_y}+\frac{1}{2}\right)\right] y \sin\left[2\pi\left(\frac{y}{L_y}+\frac{1}{2}\right)\right] = -\frac{8L_y^2}{9\pi^2}, \tag{16}$$

we finally find

$$\langle\varphi_{1,1,0}|\,\partial_y\partial_z\,|\varphi_{2,2,0}\rangle = \frac{64}{9L_yL_z}, \tag{17}$$

$$\langle\varphi_{1,1,0}|\,y\partial_z\,|\varphi_{2,2,0}\rangle = \frac{128L_y}{27\pi^2L_z}, \tag{18}$$

and so

$$C_\pm = -i\frac{64\gamma_3\hbar^2}{3\sqrt{3}L_yL_zm} \mp i\frac{128L_y\gamma_3 e\hbar B_z}{9\sqrt{3}\pi^2L_zm}. \tag{19}$$

This is the result shown in Eq. (20), considering that the Bohr magneton is $\mu_B = e\hbar/(2m)$. As explained in the above derivation, the first term on the right-hand side results from the part proportional to $\partial_y\partial_z\{J_y, J_z\}$ in the Hamiltonian H, while the second term results from the part proportional to $B_zy\partial_z\{J_x, J_z\}$.

Correction g_C to the out-of-plane g-factor

In the previous section we derived the couplings

$$C_\pm = \langle\pm3/2, 1, 1, 0|\,H\,|\pm1/2, 2, 2, 0\rangle = -i\frac{64\gamma_3\hbar^2}{3\sqrt{3}L_yL_zm} \mp i\frac{256\gamma_3L_y\mu_BB_z}{9\sqrt{3}\pi^2L_z} \tag{20}$$

assuming that the magnetic field is applied in the out-of-plane direction z. In order to calculate the associated correction g_C to the g-factor $g_\perp$, we consider a four-level system with the basis states $|3/2, 1, 1, 0\rangle$, $|-3/2, 1, 1, 0\rangle$, $|1/2, 2, 2, 0\rangle$, and $|-1/2, 2, 2, 0\rangle$ (see also Figure 4 (b) of the main article). Projection of the Hamiltonian H [Eq. (3)] onto this basis yields the effective Hamiltonian

$$H_{\text{eff}} = \begin{pmatrix} E_{g,+} & 0 & C_+ & 0 \\ 0 & E_{g,-} & 0 & C_- \\ C_+^* & 0 & E_{e,+} & 0 \\ 0 & C_-^* & 0 & E_{e,-} \end{pmatrix}, \tag{21}$$

where the asterisk stands for complex conjugation and

$$\begin{aligned} E_{g,\pm} &= \frac{\hbar^2\pi^2}{2L_z^2 m_{\text{HH}}} + \frac{\hbar^2\pi^2(\gamma_1+\gamma_2)}{2L_y^2 m} + \frac{9}{4}b(\epsilon_{zz}-\epsilon_\parallel) \\ &\quad + \frac{(\pi^2-6)(\gamma_1+\gamma_2)e^2L_y^2B_z^2}{24\pi^2 m} \pm \left(3\kappa + \frac{27}{4}q\right)\mu_B B_z, \end{aligned} \tag{22}$$

$$\begin{aligned} E_{e,\pm} &= \frac{2\hbar^2\pi^2}{L_z^2 m_{\text{LH}}} + \frac{2\hbar^2\pi^2(\gamma_1-\gamma_2)}{L_y^2 m} + \frac{1}{4}b(\epsilon_{zz}-\epsilon_\parallel) \\ &\quad + \frac{(2\pi^2-3)(\gamma_1-\gamma_2)e^2L_y^2B_z^2}{48\pi^2 m} \pm \left(\kappa + \frac{1}{4}q\right)\mu_B B_z \end{aligned} \tag{23}$$

are the energies on the diagonal. We assumed here that $\epsilon_{xx} = \epsilon_{yy} = \epsilon_\parallel$ and omitted the state-independent offset $15b\epsilon_\parallel/4$. The introduced effective masses are

$$m_{\text{HH}} = \frac{m}{\gamma_1 - 2\gamma_2}, \tag{24}$$

$$m_{\text{LH}} = \frac{m}{\gamma_1 + 2\gamma_2}. \tag{25}$$

From second-order perturbation theory,[1] we find that the low-energy 2×2 Hamiltonian obtained after diagonalization of Eq. (21) is

$$H_{\text{eff}}^{2\times 2} \simeq \begin{pmatrix} E_{g,+} - \frac{|C_+|^2}{\Delta_+} & 0 \\ 0 & E_{g,-} - \frac{|C_-|^2}{\Delta_-} \end{pmatrix}, \tag{26}$$

where we defined

$$\Delta_\pm = E_{e,\pm} - E_{g,\pm}. \tag{27}$$

With $\widetilde{\sigma}_z$ as a Pauli operator that is based on the low-energy eigenstates, Eq. (26) can be written as

$$H_{\rm eff}^{2\times2} \simeq \frac{1}{2}\left(E_{g,+} + E_{g,-} - \frac{|C_+|^2}{\Delta_+} - \frac{|C_-|^2}{\Delta_-}\right) + \frac{1}{2}\left(E_{g,+} - E_{g,-} - \frac{|C_+|^2}{\Delta_+} + \frac{|C_-|^2}{\Delta_-}\right)\widetilde{\sigma}_z. \quad (28)$$

The effective Zeeman splitting and the out-of-plane g-factor $g_\perp$ are therefore determined by

$$g_\perp \mu_B B_z \simeq E_{g,+} - E_{g,-} - \frac{|C_+|^2}{\Delta_+} + \frac{|C_-|^2}{\Delta_-}. \quad (29)$$

From Eq. (22), it is evident that

$$E_{g,+} - E_{g,-} = \left(6\kappa + \frac{27}{2}q\right)\mu_B B_z. \quad (30)$$

Given our parameters for Ge HWs, we find that the splittings $\Delta_\pm$ are predominantly determined by the confinement rather than the strain and that they can be well approximated by

$$\Delta_\pm \simeq \frac{2\hbar^2\pi^2}{L_z^2 m_{\rm LH}} - \frac{\hbar^2\pi^2}{2L_z^2 m_{\rm HH}} = \frac{\hbar^2\pi^2(3\gamma_1 + 10\gamma_2)}{2L_z^2 m} = \Delta \quad (31)$$

using $L_z \ll L_y$. With the calculated expressions for the couplings $C_\pm$ [Eq. (20)], we finally obtain

$$g_\perp \simeq 6\kappa + \frac{27}{2}q + g_C, \quad (32)$$

where

$$g_C = \frac{|C_-|^2 - |C_+|^2}{\mu_B B_z \Delta} = -\frac{2^{17}\gamma_3^2}{81\pi^4(3\gamma_1 + 10\gamma_2)} \quad (33)$$

is the correction that results from the B_z-induced difference in the tiny LH admixtures ($|\pm 1/2, 2, 2, 0\rangle$) to the eigenstates of type $|3/2, 1, 1, 0\rangle$ and $|-3/2, 1, 1, 0\rangle$. We note that $|C_\pm|/\Delta < 0.05$ for our parameters, and so the perturbation theory used in the derivation of $H_{\rm eff}^{2\times2}$ applies. Remarkably, our result for g_C depends solely on the Luttinger parameters $\gamma_{1,2,3}$.

Hamiltonian for pure heavy holes

If the contributions from LH states ($j_z = \pm 1/2$) are ignored completely, the Hamiltonian of Eq. (1) in the main text can be simplified by projection onto the HH subspace, i.e., by removing all terms that cannot couple a spin $j_z = 3/2$ (or $j_z = -3/2$, respectively) with either $j_z = 3/2$ or $j_z = -3/2$. As evident, e.g., from the standard representations of the 4×4 matrices J_ν and the 2×2 Pauli matrices σ_ν [see Eqs. (1) and (2)], this projection can be achieved by substituting $\{J_x, J_y\} \to 0$ (analogous for cyclic permutations), $J_x^3 \to 3\sigma_x/4$, $J_y^3 \to -3\sigma_y/4$, $J_z^3 \to 27\sigma_z/8$, $J_{x,y}^2 \to 3/4$, $J_z^2 \to 9/4$, $J_{x,y} \to 0$, $J_z \to 3\sigma_z/2$, which leads to the pure-HH Hamiltonian

$$\begin{aligned} H_{\mathrm{HH}} &= \frac{\hbar^2}{2m}\left[(\gamma_1 - 2\gamma_2)\, k_z^2 + (\gamma_1 + \gamma_2)\,(k_x^2 + k_y^2)\right] \\ &\quad + \left(3\kappa + \frac{27}{4}q\right)\mu_B B_z \sigma_z + \frac{3}{2} q \mu_B \left(B_x\sigma_x - B_y\sigma_y\right) + V(y,z) \end{aligned} \tag{34}$$

for the low-energy hole states in the HW. Thus, if LH states are ignored, one expects small in-plane g-factors $g_\parallel \simeq 3q \simeq 0.2$ and very large out-of-plane g-factors $g_\perp \simeq 6\kappa + 27q/2 \simeq 21.4$,[3] where we used again the band structure parameters $\kappa = 3.41$ and $q = 0.07$ of bulk Ge.[1,4]

References

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