Magnetic field effects on spin texturing in a quantum wire with Rashba spin-orbit interaction

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A quantum wire with strong Rashba spin-orbit interaction is known to exhibit spatial modulation of spin density along its width owing to coupling between subbands caused by the Rashba interaction. This is known as spin texturing. Here, we show that a transverse external magnetic field introduces additional complex features in spin texturing, some of which reflect the intricate details of the underlying energy dispersion relations of the spin-split subbands. One particularly intriguing feature is a 90° phase shift between the spatial modulations of two orthogonal components of the spin density, which is observed at moderate field strengths and when only the lowest spin-split level is occupied by electrons. Its origin lies in the fact that the Rashba interaction acts as an effective magnetic field whose strength is proportional to the electron's velocity.

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I. INTRODUCTION

Rashba spin-orbit interaction in a quantum wire can cause a multitude of spin related effects. For example, it can accumulate spin at the edges of the wire in the presence of an axial electric field, leading to the intrinsic spin Hall effect.[1–3] Even without any external electric or magnetic field, it can cause a spatial modulation of the spin density across the wire width due to subband mixing. This phenomenon has been called "spin texturing."[4–6]

Here, we study the effect of a transverse external magnetic field on spin texturing. A longitudinal magnetic field, directed along the wire axis, will affect the dispersion relations of the magnetoelectric subbands,[7,8] but a transverse magnetic field typically has more interesting effects. In addition to modifying the dispersion relations,[9,10] it can cause exotic effects such as a resonance in the spin Hall conductance.[11] Here, we show that it has nontrivial effects on spin texturing and brings out underlying features of the energy dispersion relations that usually remain concealed under equilibrium conditions. These features are observed under moderate magnetic fields and experimentally realizable conditions.

The system that we study is a semiconductor quantum wire of finite width. The transverse magnetic field is applied in the same direction as the symmetry-breaking electric field causing the Rashba interaction. We find that for weak to moderate field strength, a 90° phase shift is observed between the modulations of the spin density components along the direction of the external magnetic field and the direction of the pseudomagnetic field caused by the Rashba interaction (these two fields are mutually perpendicular). The spatial modulations of these two components are 90° out of phase with each other when only the lower spin split level in the lowest subband is occupied by electrons. When both spin-split levels in the lowest subband are occupied, other complex features emerge that reflect the intricacies of the underlying energy dispersion relations of the levels. For example, the spin density at arbitrary locations in the wire flips sign as the magnetic field is varied. This happens primarily because the energy dispersion relation of the lowest spin-split level changes dramatically as the magnetic field strength is varied. We study these effects by solving the single particle effective mass Pauli equation to find the spin eigenstates and the spin density. Finally, simple physical pictures are presented to elucidate the origin of the observed features.

II. THEORY

Consider a quantum wire with a rectangular cross section as shown in Fig. 1(a). The transverse dimension along the z direction is much larger than that in the y direction. In the Landau gauge $\vec{A}=(B_{\text{external}}z,0,0)$, the single particle effective mass Hamiltonian describing this system is

$$H=\frac{(\vec{p}+e\vec{A})^2}{2m^*}+V(y)+V(z)-\frac{g\mu_B\vec{B}_{\text{external}}\cdot\vec{\sigma}}{2}+\frac{\eta_R}{\hbar}[\sigma_z(p_x+eB_{\text{external}}z)-\sigma_x p_z], \qquad (1)$$

where g is the Landé g factor of the quantum wire material and η_R is the strength of the Rashba interaction. We ignore any spatial variation of η_R within the wire. We also ignore any band structure nonparabolicity effects which can modify the energy dispersion relations of the spin-split magnetoelectric subbands.[12,13] For the low electron energies considered in this study (low carrier concentration, only the lowest subband is occupied by electrons), these nonparabolicity effects are unimportant.

Because of the static electric field E_y inducing the Rashba interaction, the potential along $\hat{y}$ is given by $V(y)=-eE_y y$. We assume that outside $[0,W_y]$, $V(y)\rightarrow\infty$. Similarly in the $\hat{z}$ direction, we assume $V(z)=0$ for $0\leqslant z\leqslant W_z$ and ∞ everywhere else. The Rashba interaction strength η_R is related to E_y as $\eta_R=a_{46}E_y$, where a_{46} is a material constant.

The eigenenergies (E) and the corresponding two-component spinor eigenfunctions (Ψ) are found by solving the Pauli equation $H\Psi=E\Psi$, where H is given by Eq. (1).

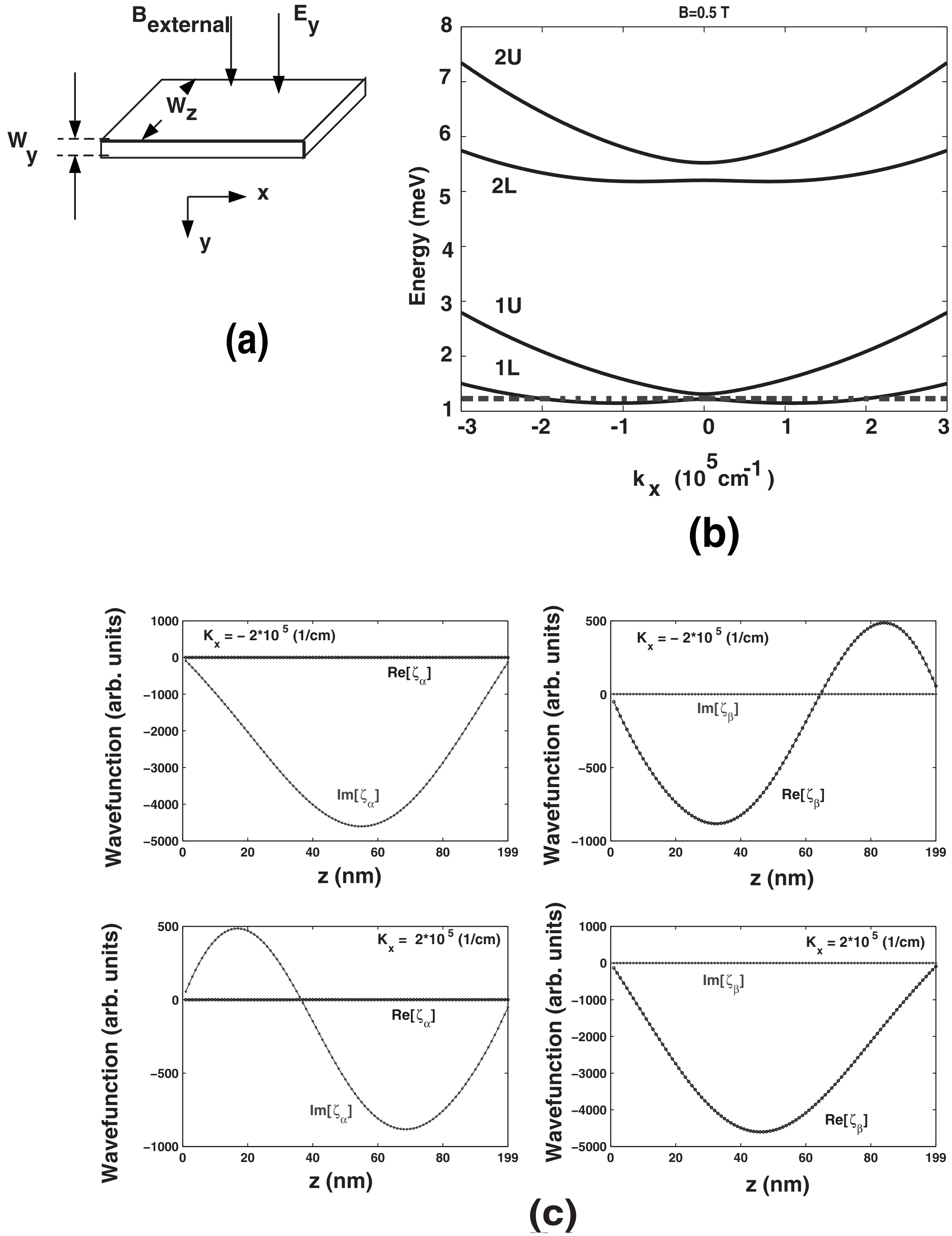

FIG. 1. (a) A quantum wire with rectangular cross section ($W_y \ll W_z = 100$ nm). A symmetry breaking electric field E_y in the y direction induces Rashba spin-orbit coupling. An external magnetic field B_{external} also acts along $\hat{y}$. (b) E-k_x plot for $B = 0.5$ T, $\eta_R = 3 \times 10^{-11}$ eV m, $m^* = 0.03 m_0$, and $g = -15$. The quantity $mL(mU)$ indicates the lower (upper) spin-split level of subband $m = 1, 2, 3., \ldots$. (c) Real and imaginary parts of the spinor wave function $\zeta(z) = [\zeta_\alpha(z) \zeta_\beta(z)]^{\mathrm{T}}$ in the $1L$ level. For negative k_x, $|\zeta_\alpha| \gg |\zeta_\beta|$ so that these states are approximately $+z$-polarized eigenspinors $[1\ 0]^{\mathrm{T}}$. For positive k_x, $|\zeta_\alpha| \ll |\zeta_\beta|$ so that these states are approximately $-z$-polarized eigenspinors $[0\ 1]^{\mathrm{T}}$. These wave functions are slightly skewed towards opposite edges for opposite signs of k_x since they are edge states.

Since the entire Hamiltonian H is translationally invariant along x and the coefficients of the Pauli matrices in H do not involve x and y variables, we can write $\Psi(x,y,z) = \exp(ik_x x)\ \phi(y)\ [\zeta_\alpha(z)\ \zeta_\beta(z)]^{\mathrm{T}}$, where the superscript "T" denotes transpose. Spatially averaging both sides of the Pauli equation over x and y coordinates, we get

$$E\zeta(z) = [H_0 I + H_s]\zeta(z), \tag{2a}$$

where

$$\zeta(z) = [\zeta_\alpha(z) \quad \zeta_\beta(z)]^{\mathrm{T}}, \tag{2b}$$

$$H_0 = \frac{\hbar^2 k_x^2}{2m^*} - \frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} + \frac{eB_{\mathrm{external}} z \hbar k_x}{m^*} + \frac{e^2 B_{\mathrm{external}}^2 z^2}{2m^*} + \epsilon_n + V(z), \tag{2c}$$

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dy^2} + V(y)\right]\phi_n(y) = \epsilon_n \phi_n(y), \tag{2d}$$

and

$$H_s = -\frac{g\mu_B B_{\mathrm{external}}\sigma_y}{2} + \eta_R\left[\left(k_x + \frac{eB_{\mathrm{external}} z}{\hbar}\right)\sigma_z + i\sigma_x \frac{d}{dz}\right]. \tag{2e}$$

Here n indicates the transverse subband index along $\hat{y}$. We assume that W_y is sufficiently small so that only the lowest subband (in the y direction) is occupied in all cases. We use the symbol m to denote the transverse subband index along $\hat{z}$.

In order to calculate the E-k_x relation and $\zeta(z)$, we solve the Pauli equation (2a) subject to the boundary conditions

$$\zeta_\alpha(z=0) = \zeta_\alpha(z=W_z) = 0,$$

$$\zeta_\beta(z=0) = \zeta_\beta(z=W_z) = 0 \tag{3}$$

using a numerical method described elsewhere.[14]

III. RESULTS

Figure 1(b) shows the typical E-k_x relationship for $B_{\mathrm{external}}=0.5$ Tesla in the presence of a Rashba interaction ($\eta_R = 3\times 10^{-11}$ eV m). The material is assumed to be InAs with effective mass $m^* = 0.03 m_0$ and $g=-15$. The horizontal axis represents $k_x + eBW_z/2\hbar$, which we refer to as k_x in the following discussion. The symbols mL and mU ($m = 1, 2, 3, \ldots$), respectively, indicate the lower and upper spin-split levels of the mth subband. Note that the lower spin-split level has a "hump" reminiscent of a camel's back. This camelback shape persists as long as the transverse field is lower than a critical value $B_{c2} = 2m^* \eta_R^2/(\hbar^2 |g| \mu_B)$, which is 0.75 T for the parameters that we have chosen. When $B_{\mathrm{external}} > B_{c2}$, the camelback feature disappears and the shape of the lower level becomes approximately parabolic like the upper level. Figure 1(c) shows the wave functions $\zeta_\alpha(z)$ and $\zeta_\beta(z)$ for $k_x = \pm 2\times 10^5$ cm^{-1} in the $1L$ subband when $B_{\mathrm{external}} = 0.5$ T. As expected, these wave functions are skewed towards the edges of the wire, characteristic of "edge states."

We define spin components $\mathcal{S}_j^m(k_x,z)$ in the mth level as

$$\mathcal{S}_j^m(k_x,z) = \frac{[\zeta_{\alpha,m}^*(k_x,z) \quad \zeta_{\beta,m}^*(k_x,z)]\sigma_j[\zeta_{\alpha,m}(k_x,z) \quad \zeta_{\beta,m}(k_x,z)]^{\mathrm{T}}}{|\zeta_{\alpha,m}(k_x,z)|^2 + |\zeta_{\beta,m}(k_x,z)|^2}, \quad j = x,y,z, \tag{4}$$

where $[\zeta_{\alpha,m}(z)\ \zeta_{\beta,m}(z)]^{\mathrm{T}}$ is the spinor wave function in the mth spin-split level.

The above quantities not only depend on k_x, but depend on z as well. An electron, with a fixed k_x and belonging to a particular subband (mL/U), has different spin orientations depending on its physical location along the width of the quantum wire channel.

In order to find the net spin polarization density as a function of the z coordinate, we compute the quantity

$$S_j(z) = \sum_m^M \frac{\int_{k_{Fm}^-}^{k_{Fm}^+} \mathcal{S}_j^m(k_x,z)dk_x}{k_{Fm}^+ - k_{Fm}^-}, \quad j = x,y,z, \tag{5}$$

where M is the number of occupied spin-split levels (whose bottoms are below the Fermi energy) and k_{Fm}^+ (k_{Fm}^-) is the wave vector in the mth level where the Fermi level intersects the E-k_x curve on the right (left). Here, we have assumed that the temperature is low enough that the electron occupation probability, which is the Fermi-Dirac factor, can be approximated as $\Theta(E-E_F)$, where Θ is the Heaviside function. If the E-k_x curve is symmetric about the energy axis, then $k_{Fm}^+ = -k_{Fm}^-$; otherwise (as in the case of $B=0$, when the E-k_x relations in the lowest subband are two horizontally displaced parabolas), $k_{Fm}^+ \neq -k_{Fm}^-$. A special case arises when $B < B_{c2} = 2m^* \eta_R^2/(\hbar^2|g|\mu_B)$ and the E-k_x curve has a camelback shape. If the Fermi level is below the "hump" of the camelback, then

$$S_j(z) = \frac{\int_{k_{F1}}^{k_{F2}} \mathcal{S}_j(k_x,z)dk_x}{k_{F2} - k_{F1}} + \frac{\int_{k'_{F1}}^{k'_{F2}} \mathcal{S}_j(k_x,z)dk_x}{k'_{F2} - k'_{F1}}. \tag{6}$$

Here k_{F1}, k_{F2} are the wave vectors where the Fermi level intersects the E-k_x curve on the left of the energy axis, and k'_{F1}, k'_{F2} are the wave vectors where the Fermi level intersects the E-k_x curve on the right of the energy axis. Note that because of ensemble averaging in Eqs. (5) and (6) (represented by integration over the k states), the norm of $S(z)$ is not conserved, i.e.,

$$S_x^2(z) + S_y^2(z) + S_z^2(z) \neq 1 \tag{7}$$

at any arbitrary z coordinate.

In Fig. 2, we plot $S_x(z)$, $S_y(z)$, and $S_z(z)$ as a function of the z coordinate when $B_{\mathrm{external}}=0.5$ and 10 T, while maintaining a constant Rashba spin-orbit interaction strength $\eta_R = 3\times 10^{-11}$ eV m. The carrier concentration in the wire is kept fixed at 6.3×10^4 cm^{-1}. For this small carrier concen-

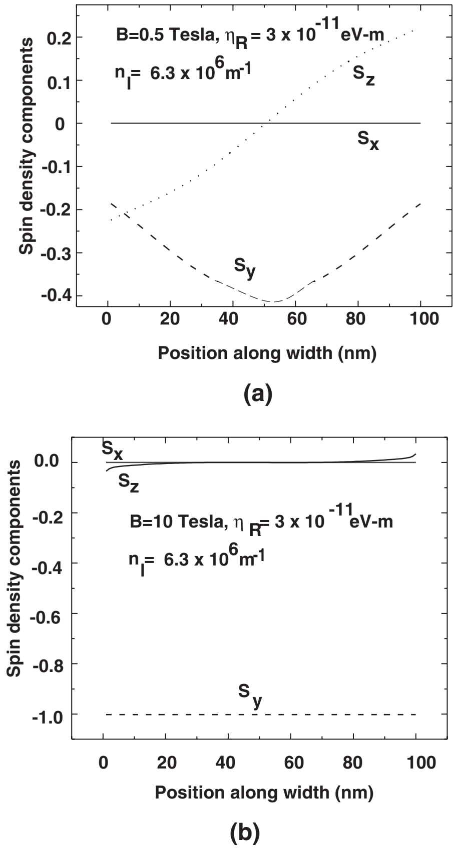

FIG. 2. The spin polarization density $S_x(z)$, $S_y(z)$, and $S_z(z)$ as a function of the z coordinate for two different values of B_{external}: (a) 0.5 T and (b) 10 T. The strength of the Rashba interaction $\eta_R=3\times10^{-11}$ eV m. The electron density is kept fixed at 6.3×10^4 cm^{-1} and only the lower spin-split level is occupied.

tration, only the lower level $1L$ is occupied (at 0 K). The upper level $1U$ is unoccupied since the Fermi level always happens to be below it.

In Fig. 2, we did not show the spatial variation of $S_x(z)$, $S_y(z)$, and $S_z(z)$ when $B_{\text{external}}=0$ since then there is no significant spatial modulation. Without an external magnetic field, $S_x(z)=0$ and $S_y(z)=S_z(z)\approx 0$ for all z. To see any strong spatial modulation in the absence of an external magnetic field (i.e., significant spin-texturing),[4] we need very strong coupling between the subbands, which we do not have in our case. Our wire width is small enough that the energy spacing between subbands is large and intersubband coupling is small.

Returning to Fig. 2(a), we find that when $B_{\text{external}}=0.5$ T, $\langle S_x\rangle=0$ everywhere in all cases, but there is a clear spatial modulation in S_y and S_z along the z axis. This results in a standing "half wave" along the wire width. What is interesting is that there is a $\pi/2$ *phase shift* between the spatial modulations of S_y and S_z, i.e., the y and z components of the spin density modulations are 90° out of phase with each other.

We provide a simple (qualitative) physical picture to explain the origin of this phenomenon. The Rashba spin-orbit interaction gives rise to an effective magnetic field B_{Rashba}.[15] It is directed along the z axis, since it must be along a direction that is mutually perpendicular to the symmetry breaking electric field inducing the Rashba effect (which is along the y direction) and the electron's velocity (which is along the x direction). This field B_{Rashba} is proportional to the electron's translational velocity v_x along the wire axis.

When a y directed external magnetic field is present (i.e., $B_{\text{external}}\neq 0$), electrons in the center of the wire will be in closed Landau orbits on the x-z plane with no translational velocity ($\langle v_x\rangle=0$). Therefore they experience no B_{Rashba}. However, electrons at the edges of the wire are in "edge states" and have nonzero translational velocity ($\langle v_x\rangle\neq 0$). As a result, they experience a nonzero B_{Rashba}. Furthermore, since electrons at opposite edges have oppositely directed velocities, they will experience oppositely directed B_{Rashba}.

Therefore the net magnetic field that electrons experience in the wire is *entirely* y directed at the center since B_{Rashba} is zero there. At the edges, $B_{\text{Rashba}}\neq 0$, so that the net magnetic field there has both a y component and a z component. Since the z component of the spins will line up parallel to B_{Rashba} and produce a net z polarization of spins, we expect that $S_z(z)$ will be zero at the center of the wire (because the Rashba field is zero at the center), maximum at the edges, and have opposite signs at the two edges because edge states at the two edges have oppositely directed translational velocities. At the same time, S_y will be maximum at the center and minimum at the edges since the net effective magnetic field is entirely y directed at the center, but not away from the center. This is precisely what we see and this is also the explanation for the $\pi/2$ phase shift between the y and z components of the spin density modulation. The $\pi/2$ phase shift is simply a manifestation of the fact that $|S_z|$ is minimum at the center and maximum at the edges, while $|S_y|$ is maximum at the center and minimum at the edges. Note that S_y is always negative because of the negative g factor ($g=-15$ for InAs) assumed in the calculations.

There is never any x component of magnetic field seen by any electron under any circumstance. Therefore $S_x(z)$ is always zero at every z coordinate.

If B_{external} is too strong (10 T), then it completely overwhelms the relatively puny B_{Rashba}. Furthermore, most electrons then condense into closed Landau orbits with no translational velocity, so that they experience no B_{Rashba} in any case. Therefore the overwhelmingly dominant magnetic field every electron experiences is the strong y-directed external field. Consequently, *every* spin aligns antiparallel to B_{external} (i.e., along the negative y axis) everywhere except at the very edges where there may be some lingering vestigial B_{Rashba} due to any surviving edge state with nonzero translational velocity. Consequently, $S_z=0$ all along the width, except perhaps at the very edges, and $S_y=-1$ (except at the very edges) since the external field is very strong and forces every spin to align antiparallel to it. This is what we see in Fig. 2(b). Furthermore, since B_{external} is spatially *invariant* unlike B_{Rashba}, it ends up quenching the spatial modulation of the spin density when it is very strong.

In Figs. 3(a) and 3(b), we plot $S_y(z)$ and $S_z(z)$ as a function of z for different magnetic fields. Note that the $\pi/2$ phase shift feature between the spatial modulation of $S_y(z)$ and $S_z(z)$ is preserved at all magnetic fields.

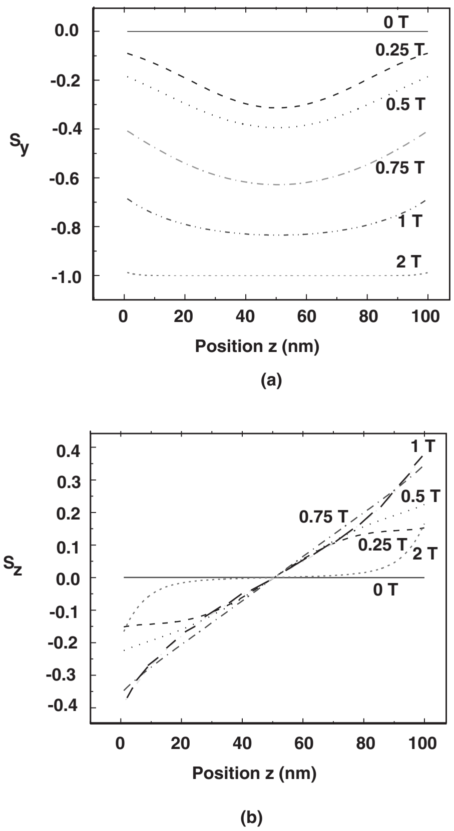

FIG. 3. The spin polarization density (a) $S_y(z)$ and (b) $S_z(z)$ as a function of the z coordinate for different values of B_{external}. The strength of the Rashba interaction $\eta_R = 3\times10^{-11}$ eV m. The electron density is kept fixed at 6.3×10^4 cm^{-1} and only the lower spin-split level is occupied.

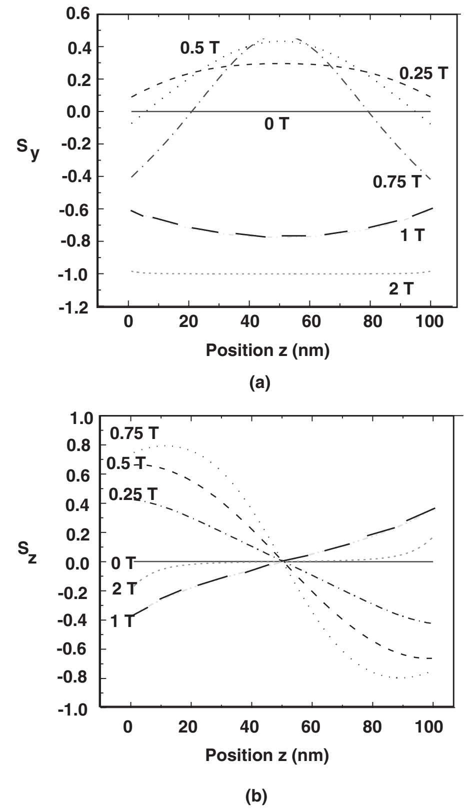

FIG. 4. The spin polarization density (a) $S_y(z)$ and (b) $S_z(z)$ as a function of the z coordinate for different values of B_{external}. The strength of the Rashba interaction $\eta_R = 3\times10^{-11}$ eV m. The electron density is kept fixed at 9.2×10^4 cm^{-1} and only the lower spin-split level is occupied when $B_{\text{external}} < 0.75$ T. Under weaker magnetic fields, both lower and upper spin-split levels are occupied.

In Figs. 4(a) and 4(b), we plot $S_y(z)$ and $S_z(z)$ as a function of z for different magnetic fields when the carrier concentration in the wire is increased to 9.2×10^4 cm^{-1}. For this carrier concentration, both spin-split levels ($1L$ and $1U$) of the lowest subband are occupied as long as B_{external} is less than some critical field B_{c1}. As B_{external} is increased, the spin splitting between the $1L$ and $1U$ levels increases. Ultimately, when $B_{\text{external}} > B_{c1}$, the upper spin-split level ($1U$) depopulates and only the lower level ($1L$) is occupied.

As long as a single subband ($1L$) is occupied, i.e., when $B_{\text{external}} > B_{c1}$, the features in Fig. 4 are the same as in Fig. 3, as expected. However, when $B_{\text{external}} \leq B_{c1}$ so that *both* spin-split levels are occupied, there is a *sign reversal* in $S_z(z)$, meaning that at any location $z = z_0$, the sign of $S_z(z)$ is opposite to what it is when a single spin-split level is occupied. The quantity $S_y(z)$ has an even more complex behavior. When the external field is very weak (0.25 T), $S_y(z)$ is positive everywhere, i.e., the y component of the spins are lining up *parallel* to the y-directed external field despite the fact that the g factor is negative. At stronger magnetic fields (0.5 and 0.75 T), there are zero crossings. The y component of the spins are lining up parallel to the external field near the wire's center, but antiparallel near the edges.

These are nontrivial effects of the energy dispersion relations of the two spin-split levels. When both levels are occupied, they both contribute to $S_z(z)$ and $S_y(z)$, but typically with opposite signs. Since at any given k state, the spin eigenstates in these two levels are orthogonal, the contributions to either $S_z(z)$ or $S_y(z)$ from the two levels tend to have opposite signs. As a result, there can be some *cancellation* between their contributions. If the upper level $1U$ dominates, then we will get one particular sign of $S_z(z)$ or $S_y(z)$ at a given location $z = z_0$, whereas if the lower level dominates, we will get the opposite sign.

Normally, one would expect the lower level $1L$ to dominate, since it has the higher occupation probability; but this does not always happen. The electron density is given by $\int D(E)f(E)dE$, where $f(E)$ is the occupation probability (Fermi Dirac factor) and $D(E)$ is the density of states. When B_{external} is less than B_{c2}, the lower level $1L$ has a "camelback" shape so that the density of states in this level has a complicated energy dependence. As a result, depending on the placement of the Fermi level (i.e., the carrier concentration), this level can contain fewer electrons than the $1U$ level even though it has the higher occupation probability. Furthermore, electrons in the lower level tend to have lower velocities because of the nonmonotonic energy-wave-vector relation, and thus experience a smaller z component of B_{Rashba} on the average. Therefore the $1L$ level may contribute less to S_z than the $1U$ level as long as $B_{\text{external}} < B_{c2}$. In that case, the

$1U$ level will dominate and the sign of $S_z(z)$ and $S_y(z)$ will be determined by the $1U$ level. If this happens, then the sign of $S_z(z)$ and $S_y(z)$ will be opposite to what they would be if only one level (the $1L$ level) were occupied.

When B_{external} is increased, two effects can occur. First, the camelback shape in the $1L$ level will disappear when B_{external} exceeds B_{c2}. After that, the shape of the $1L$ level will begin to resemble that of the $1U$ level. When this happens, the $1L$ level takes over the dominant role and becomes the major (albeit not the sole) contributor to $S_z(z)$ because it has the higher occupation probability. The second effect is that when the magnetic field is increased, the energy splitting between the $1L$ and $1U$ level increases. At some point, when B_{external} exceeds a critical value B_{c1}, the $1U$ level gets completely depopulated and the $1L$ level becomes the sole contributor to $S_z(z)$. Suffice it to say then that as we vary B_{external}, we expect to see a change in the sign of $S_z(z)$ because of a swapping of the dominant role between the $1L$ and $1U$ levels.

This is precisely what we see in Fig. 4. In this case, a change in sign of $S_z(z)$ occurs around 0.75 T which happens to be the value of both B_{c1} and B_{c2} because of the parameters that we have chosen in this study. In reality, the change of sign will occur when B_{external} exceeds B_{c1} or B_{c2}, whichever is smaller.

The effect of the energy dispersion relations is even more pronounced in the behavior of $S_y(z)$. When the magnetic field is 0.25 T, the $1U$ level dominates. Since the g factor is negative, the y component of the spins will align parallel to B_{external} in the $1U$ level and antiparallel in the $1L$ level. Because of the dominance of the $1U$ level (since $B_{\text{external}} < B_{c1}, B_{c2}$), the y component of the net spin polarization is parallel to B_{external} and $S_y(z)$ is positive throughout. As we increase the magnetic field, the dominance of the $1U$ level wanes. At 0.5 T and 0.75 T, the sign of $S_y(z)$ is negative near the edges of the wire, but positive around the center. This highlights the fact that the relative contributions of the $1L$ and $1U$ levels to either $S_z(z)$ or $S_y(z)$ depend on the z coordinate, as should be evident from Eq. (5) or Eq. (6).

In conclusion, we have studied the effect of a transverse magnetic field on spin density modulation in a quantum wire with strong Rashba coupling. We have explained why a moderate magnetic field introduces a $\pi/2$ phase shift between the modulations of the spin density components along the external magnetic field (y direction) and along the direction of the effective magnetic field due to Rashba interaction (z direction). We have also highlighted the intricate influence of the underlying energy dispersion relations of the spin-split subbands on the spin density modulation.

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