Strong Dependence of Spin Direction and Wave Function Localization on In-plane Wave Vector in Wide Modulation-doped Quantum Wells

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Abstract. An important mechanism in spintronics is spin-splitting induced by structure and/or bulk inversion asymmetry. These effects are frequently assumed to depend on two parameters usually denoted by $\alpha$ and $\beta$, respectively, and $\alpha$ is assumed to be proportional to some average electric field. We here demonstrate that the spatial dependence of the electric field gives very important effects absent in simpler models. These effects are particularly clear in wide modulation-doped quantum wells where there are two weakly interacting electron gases in the interface regions. Using an $8 \times 8$ $k \cdot p$ matrix approach we obtain anticrossings between interacting subbands at which the spin direction and/or wave function localization are found to be strong functions of the in-plane wave vector.

1. Introduction

A rapidly growing research field is called spintronics in which the spin of the carriers is utilized to obtain new functionalities. A convenient way to control the spin splitting of subbands in a quantum well is to utilize the Rashba effect [1] in which an applied or built-in macroscopic electric field gives rise to structure inversion asymmetry (SIA) which together with spin-orbit interaction gives rise to spin splitting even in the absence of magnetic field or magnetic atoms. This effect is frequently described by the Rashba term

$$H_R = \alpha \sigma \cdot k \times n$$

(1)

Here $\alpha$ is called the Rashba parameter which is usually taken to be proportional to some average electric field, e.g. the expectation value of the electric field. $\sigma$ is given in terms of Pauli matrices, $k$ is the wave vector and $n$ is the unit vector in the direction of the electric field, which we take to be the $z$-direction, perpendicular to the interfaces of the quantum well structure. In this case Eq. (1) becomes

$$H_R = \alpha(\sigma_x k_y - \sigma_y k_x)$$

(2)
The Rashba term describes the spin splitting of an isolated electron subband well, but when we have interacting electron subbands or hole subbands [2] it turns out to be important to use a more accurate matrix approach.

Spin splitting can also occur because of the inversion asymmetry of the zincblende crystal called bulk inversion asymmetry (BIA). The resulting spin splitting is called the Dresselhaus effect [3] and is usually described by terms linear in $k$

$$H_D = \beta (\sigma_y k_y - \sigma_x k_x)$$

(3)

This common approach has the advantage that one can easily obtain analytical expressions for the total effect of $H_R$ and $H_D$, but it should be noted that both of these terms represent lowest order approximations [4]. The effects that we obtain in an 8-band $k\cdot p$ approach [4] would not appear in common simpler approaches. We include the interaction between the conduction, heavy-hole, light-hole and split-off bands exactly and the remote bands in perturbation theory.

2. Method

We have performed self-consistent subband structure calculations for modulation-doped In$_{0.74}$Ga$_{0.26}$Sb quantum wells surrounded by In$_{0.7}$Al$_{0.3}$Sb barriers. The spin-orbit interaction of these materials is almost as strong as that of InSb and we can choose the Ga and Al contents to give lattice match and a suitable conduction band offset. In this paper we take the well width to be 80 nm, the spacer layers 44 and 46 nm and the donor concentration $2.5 \times 10^{17}$ cm$^{-3}$ which gives an electron density of $6 \times 10^{11}$ cm$^{-2}$. We here consider wave vectors $k$ along the [11] direction in the two-dimensional Brillouin zone.

In this way we essentially obtain two weakly interacting electron gases at the two interfaces. With the well width, spacer layers and a possible applied electric field we can easily control the degree of asymmetry and the interaction between the electron gases. The small asymmetry in our case gives a small energy difference at $k = 0$ between the lowest and next lowest subband pairs and produces the anticrossing phenomena described below.

3. Results

At $k = 0$ the lowest subband pair has wave functions with larger amplitude in the left interface region, where the potential is deeper but with non-negligible amplitude at the right interface. The second subband pair is separated from the first by $E_{21} = 1.45$ meV and has the larger wave function amplitude to the right. For finite $k$ each subband splits up into what we denote two spin subbands. For a given $k$ we number them in order of increasing energy. The interaction between the spin subbands gives rise to several intricate anticrossings.

3.1. Wave function interchange at $k \approx 0.03$ nm$^{-1}$. In the Rashba model the energy spin splitting $\Delta E$ increases linearly with $k$ and it is clear that for sufficiently large $k$ it would become larger than $E_{21}$. If the subbands were treated as noninteracting the spin subbands 2 and 3 (corresponding to the upper and lower component of the lowest and next lowest subband pair, respectively) would cross. In our approach we instead obtain anticrossing (avoided crossing). In such cases the anticrossing spin subbands tend to interchange identities. In our case spin subband 2 moves from the left to the right and spin subband 3 moves in the opposite direction as $k$ is increased. This process occurs gradually and near $k = 0.03$ nm$^{-1}$ the squared wave functions are distributed equally between the interface regions. This has been described elsewhere [5].

If we label the lower spin subband of the lowest subband pair by “spin up” and its upper spin subband by “spin down” it should be noted that we should use the opposite labels for the next lowest subband pair since the sign of the electric field differs between the two interface regions. Thus the spin subbands 2 and 3 have the same spin label and it is also found in our calculations that the spin properties are not changed significantly during this anticrossing process.
3.2. Wave function and spin interchange at \( k = 0.168 \text{ nm}^{-1} \). A much more rapid interchange of properties occurs at the anticrossing between the lowest two spin subbands 1 and 2 when \( k \) is increased from 0.166 to 0.170 nm\(^{-1}\). As is shown in the upper part of Fig. 1 a-c the wave function of spin subband 1 rapidly moves from the left to the right while that of spin subband 2 (lower part) moves in the opposite direction. Simultaneously the spin expectation values \([4]\) have their directions reversed as is shown in the insets. To understand this behaviour it is important to note the effect of the first anticrossing described in subsection 3.1. After this the second spin subband has retained the opposite spin direction compared to spin subband 1 but is now localized to the right interface. Because of the weak interaction between these spin subbands with opposite spins and wave function localizations they reach a minimal energy separation of only 0.43 meV at \( k = 0.168 \text{ nm}^{-1} \) where the wave functions are seen to be distributed evenly between the interface regions and the spin projection in the \( xy \)-plane is small (Fig. 1 b). Such a weak interaction yields a property interchange taking part over quite a small \( k \)-interval. We have found that the Dresselhaus terms are essential to obtain this behaviour. It can be noted that after this anticrossing the lowest spin subband is localized to the right although the potential is lower to the left.

Fig. 1. Squared wave functions for lowest (upper part) and next lowest (lower part) spin subband for three values of the in-plane wave vector \( k_{\parallel} \). Insets: projection of the spin vector in the \( xy \)-plane.

3.3. Spin interchange at \( k \approx 0.30 \text{ nm}^{-1} \). A third kind of anticrossing occurs near \( k = 0.30 \text{ nm}^{-1} \) between spin subbands 2 and 3. After the two earlier anticrossings these two spin subbands actually have properties similar to the initial lowest subband pair for small \( k \): opposite spin directions and both wave functions localized to the left. As is seen in Fig. 2 this anticrossing is rather peculiar and actually takes place in two steps. In the lower part we have shown the projection in the \( xy \)-plane of the expectation value of the spin vector for a succession of \( k \)-values. At \( k = 0.292 \text{ nm}^{-1} \) the \( y \)-component changes sign rapidly while the \( x \)-component makes a rapid sign change at \( k = 0.317 \text{ nm}^{-1} \) such that the spin direction for \( k > 0.317 \text{ nm}^{-1} \) becomes opposite of what it was for \( k < 0.292 \text{ nm}^{-1} \). In this range the \( z \)-component (not shown) becomes unusually large and rapidly varying with absolute values comparable to the \( x \)- and \( y \)-components while they usually are much smaller. During this process the energy separation is much more slowly varying than for the surrounding \( k \)-values with a minimum value of 0.007 meV as is seen.
in the upper part of Fig. 2. For $k$-values beyond this anticrossing the two lowest spin subbands have the same spin direction and it becomes non-trivial how one should define the spin splitting. This yields an interesting relation to the spin Hall effect that will be discussed elsewhere.

Fig. 2. Lower part: Projection of spin vector in the $xy$-plane for spin subband 1 for a succession of $k$-values. Vertical scale: $y$-component, horizontal scale: $x$-component. Spin subband 2 has the opposite qualitative behaviour. The upper part shows the energy separation between the lowest spin subbands for the same $k$-values. The inset shows this spin subband separation on a larger scale.

4. Discussion

Wide modulation-doped quantum wells display both useful and interesting properties. We have recently shown [5] how one can enhance the Rashba effect at a given bias by an order of magnitude by utilizing the strong electric fields at the interfaces. Instead of applying a strong electric field it is sufficient to apply an electric field that barely causes the wave functions to be localized to one of the interface regions where the electrons “feel” the interface field rather than the average field. This requires a somewhat stronger electric field than considered in this work and can give an improved version of the Datta-Das spin transistor [6]. The fact that the electric fields have different signs at the two interfaces implies that the direction of the spin precession is different in the two electron gases, but this does not preclude the possibility of constructive or destructive interference on the arrival at the drain of the spin transistor. Although the situation with several filled spin subbands is more complicated than the spin transistor originally proposed by Datta and Das [6] wide modulation-doped quantum wells provide a novel means of switching between a symmetric and a slightly asymmetric quantum well with a bias that is an order of magnitude smaller than with a uniform electric field in the quantum well. Assuming that the switch energy is proportional to $CV^2$, where $C$ is the capacitance of the device and $V$ is the bias, this mechanism could reduce the switch energy by two orders of magnitude and make them competitive with state-of-the-art Si MOSFETs. (Cf. ref. [7]).

The effects of anticrossings are interesting but their usefulness is not immediately clear and deserves further studies. For a symmetric potential it is well known that the two lowest subbands have
symmetric and antisymmetric wave functions, respectively. For small asymmetry rapid anticrossings were seen to take place as the in-plane wave vector increased. If the transport in a spin subband can be considered as adiabatic, this can possibly yield observable effects. For device aspects it is desirable to make spin flips with a small variation of some external parameter like the applied electric field. It seems likely that one can design a structure where the anticrossing behaviour is achieved as the electric field is increased slightly such that the spin direction at the Fermi energy of a spin subband is flipped. It is conceivable that the electric field required for this process is much smaller than that required for spin precession by $\pi$ in the original spin transistor [6]. A complication is that at anticrossings the opposite trend occurs for an adjacent spin subband and the individual effects may be hard to distinguish. But since this spin flip can occur in spatially separated electron gases interesting and possibly useful effects can be envisioned, especially if one manages to contact the two interface regions separately. This spatial separation by a barrier about 100 meV high could also make devices less sensitive to elevated temperatures in spite of the small energy separations between the involved spin subbands.

In the common Rashba model the spin splitting is usually assumed to be proportional to the expectation of the electric field. Then one implicitly assumes that this expectation value is the same for both the spin subbands of the subband pair. The interchange of wave functions at anticrossings demonstrates that this assumption can be wrong and that this procedure is not always well defined. Our numerically calculated expectation values at the Fermi energy show that the expectation values even can have opposite signs for the components of a subband pair. Furthermore, even in the case of an electric field sufficiently strong that the wave functions are almost entirely localized to one interface region and the two expectation values are approximately equal we have found that inserting the average expectation value of a subband pair into the Rashba term underestimates the spin splitting by a factor two compared to our numerical calculations.

We have implicitly assumed that the wave functions are coherent over the whole quantum well in spite of the high electrostatic barrier essentially separating the electron gases. It should depend on the quality of the sample if this assumption holds. The system we have considered with the anticrossing phenomena seems to be ideal for further studies of these fundamental issues.

5. Conclusions

In conclusion we have demonstrated that interesting anticrossing phenomena can occur in slightly asymmetric wide modulation-doped quantum wells. We have shown examples of three fundamentally different anticrossing cases. In one case the wave functions of two anticrossing spin subbands are interchanged as the in-plane wave vector is increased while the spin properties are not affected. For large $k$ the opposite effect occurs and the spin flip is actually found to occur in two steps, first the $x$-component is reversed and then the $y$-component for a slightly larger $k$-value. For an intermediate $k$-value both wave function interchange and spin flip occur over a very small range of $k$-values. Inclusion of Dresselhaus terms is important for obtaining the anticrossing behaviour in some cases. For somewhat larger asymmetry a very efficient switch mechanism for a Datta-Das-like spin transistor is demonstrated.

References
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