Spin mixing between subbands and extraordinary Landau-level shift in wide HgTe quantum wells

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We present both the experimental and theoretical investigations of a nontrivial electron Landau-level shift in magnetic field in wide (~20 nm) HgTe quantum wells: Landau levels split under magnetic fields but become degenerate again when magnetic field increases. We reproduced this behavior qualitatively within an isotropic six-band Kane model; then using semiclassical calculations, we showed this behavior is due to the mixing of the conduction band with a total spin of $3/2$ with the next well subband with a spin of $1/2$, which reduces the average vertical spin from $3/2$ to around 1. This change in the average spin changes the Berry phase, explaining the evolution of Landau levels under magnetic field.

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I. INTRODUCTION

The recent discovery of topological insulators, a new state of mater, in materials with strong spin-orbit interaction [1–6] has opened an exciting research direction. In most topological insulators the strong relativistic effects and, particularly, spin-orbit coupling lead to an inverted spectrum which is at the origin of their topological properties. Since relativistic effect strength grows with increasing atomic mass, investigations have focused on a broad range of materials with Bi and Sb [7–11], InAs/(In)GaSb [12–14], and HgTe [3,15,16] quantum wells, all containing elements with large atomic numbers in the Mendeleev periodic table. The quantum wells based on HgTe and InAs/GaSb can be grown epitaxially, and the carrier density can be tuned with a gate in a broad range; these systems are thus particularly suited to fundamental investigations on topological insulators. One of the principal features of HgTe quantum wells is that their properties drastically depend on their thickness. By changing the width d of the quantum well [17] one can get an ordinary insulator like GaAs quantum wells at $d < 6.3$ nm [2,3,15], a linear spectrum of so-called Dirac fermions at the critical thickness $d \approx 6.3$ nm [18,19], an inverted spectrum of two-dimensional (2D) topological insulators at $d > 6.3$ nm [2,3,15,16], a 2D semimetallic spectrum with a small overlap between the conduction and valence bands at $d \approx 20$ nm [20,21], and the spectrum of a three-dimensional topological insulator at width $d > 70$ nm [22–24]. For the last two cases the well should be strained; this is achieved by a lattice mismatch between HgTe and CdTe.

In addition to its impact on the band structure, spin-orbit interaction can appear directly in magnetotransport experiments through the shift of the Landau levels (LL). Previous works [25–27] focused on Landau-level shift due to Rashba splitting arising as a consequence of the asymmetric deformation of the quantum well at high gate voltages. In this work we present magnetotransport experiments and a thorough theoretical analysis showing that the shift of the Landau levels can also occur due to mixing of quantum well subbands with different spins. Indeed, the average spin of the quantum well wave function is directly connected to the Berry phase since both describe the transformational properties of the wave function under plane rotation. The change in the wave function spin thus directly leads to an anomalous shift of the Landau levels due to the contribution of the Berry phase to the semiclassical quantization rule for Landau levels [28–36]. Following these theoretical works, we develop a quantitative semiclassical model which reproduces the Landau levels obtained numerically in a realistic six-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory calculation; these theoretical results are then compared to the experiment.

II. EXPERIMENT

Our experiments were carried out on 20–22-nm undoped $Cd_{0.6}Hg_{0.4}Te/HgTe/Cd_{0.6}Hg_{0.4}Te$ heterostructures with (013) surface orientation, grown by molecular beam epitaxy. The cross section of the structures is illustrated in Fig. 1(a). A detailed description of sample preparation can be found in [21,37]. These quantum wells have a separation of 65 meV between p-like well conduction subband [H1] with a total spin (angular momentum) of $3/2$ and the first excited s-like subband [E2] with a spin of $1/2$. This splitting is sufficiently large to resolve a large number of Landau levels in the conduction band at few-tesla magnetic fields but still within the range covered by changes in the gate potential; 20–22-nm-wide quantum wells were thus optimal for our experiments. The evolution of the conduction band spin as a function of momentum k is shown in the inset in Fig. 1(b); the average spin in the z direction indeed changes from $3/2$ at low energies to around 1 near the bottom of subband [E2] as a consequence of their mixing. The previous works on similar HgTe samples [20,38–43] mostly concentrated on the energy region where the conduction and valence bands overlap [see Fig. 1(b)], leading to the coexistence of electrons and holes. It has been shown in InAs/GaSb quantum wells [44] that mixing between p-like electron and s-like hole states can already lead to a nontrivial LL behavior. In our case both

