Absence of magneto-intersubband scattering in *n*-type HgTe quantum wells

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Magneto-intersubband scattering (MIS), which is a general feature in III-V semiconductor heterostructures with two occupied subbands, is demonstrated to be absent in both asymmetric and symmetric type-III HgTe quantum wells (QW's). The analysis of the temperature dependence of Shubnikov–de Haas (SdH) oscillations and their fast Fourier transforms, together with the excellent agreement between the measured longitudinal resistivity and the calculated oscillations in the density of states in a magnetic field within the framework of an 8×8 $\mathbf{k}\cdot\mathbf{p}$ model, completely rule out the MIS effect. The absence of the MIS effect in HgTe QW's is ascribed to a much more complex and irregular Landau level alignment which suppresses the intersubband scattering rate. A natural consequence of the absence of MIS is that the Rashba spin splitting can be properly identified from the SdH oscillations in a perpendicular magnetic field and at a constant temperature, in contrast to the recent findings for InAs QW's.

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I. INTRODUCTION

The observation of an enhancement of the intersubband scattering in some III-V heterostructures with two occupied subbands in a perpendicular magnetic field has aroused much interest. Leadley *et al.*[1] first reported an increased temperature-dependent modulation of two sets of Shubnikov–de Haas (SdH) oscillations for a GaAs/AlGaAs heterojunction, which was initially attributed to acoustic-phonon-assisted intersubband scattering. However, later measurements[2–5] show that the intersubband scattering is not temperature dependent below 20 K. The concept of resonant elastic intersubband scattering was first proposed by Polyanovsky[6] and Leadley *et al.*[7] and was later named the magneto-intersubband scattering (MIS) effect by Raikh and Shahbazyan.[8] It is schematically shown in Fig. 1. If both subbands are parabolic, have equal effective masses m^*, and their energy separation is E_{10}, then at some particular magnetic fields, when $\Delta E_{10}=p\hbar\omega_c$, where p is the integer indicated in the boxes of Fig. 1, the two sets of Landau levels will be perfectly aligned, as shown by the dotted lines in Fig. 1. This will result in an enhancement of the elastic intersubband scattering rate and hence a new oscillation frequency in the magnetoresistance with a period of $\delta(1/\hbar\omega_c)=1/\Delta E_{10}$. Raikh and Shahbazyan[8] gave a thorough theoretical treatment for the magnetoconductivity for a two-subband two-dimensional electron gas (2DEG) which includes SdH and MIS using the self-consistent Born approximation generalized to the case of two subbands. Since MIS is related to the alignment of the two sets of Landau levels and not dependent on Fermi energy E_F, it should exhibit negligible sensitivity to temperature.[8–11] The temperature damping of the SdH oscillations and temperature insensitive MIS oscillations result in an increased degree of modulation with increasing temperature as mentioned above.[8] A phase shift of π between MIS and SdH has been found by Sander *et al.*[9] in an AlGaAs/InGaAs/GaAs quantum well (QW) when the Fermi energy lies at the bottom of the second subband. The absolute amplitude of MIS conductivity has recently been calculated by Averkiev *et al.*[12]

In asymmetrically doped narrow-gap semiconductor heterostructures, the situation becomes more complex because of the presence of Rashba spin splitting, which is the lifting of spin degeneracy due to the asymmetric confinement potential in semiconductor heterostructures with strong spin-orbit interaction.[13] It has been extensively studied both experimentally[14–18] and theoretically.[19,20] Recently, the origin of the beat patterns in the magnetoresistance of InAs QW's with two populated subbands has been investigated by Rowe *et al.*[11] They argue that, in asymmetric QW's with two occupied subbands, the mixing of the first subband SdH series and MIS oscillations will lead to a beating effect, which has been ascribed to the Rashba spin splitting in the literature. Consequently, the authors conclude that *measurements of the SdH oscillations, in the presence of two occupied sub-*

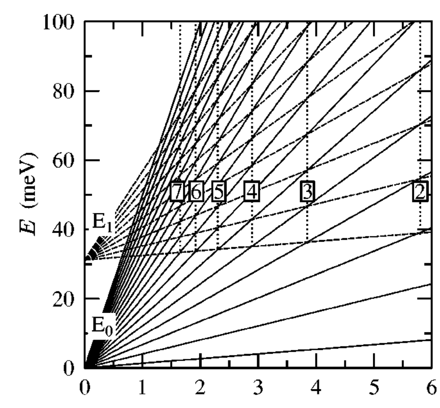

FIG. 1. A schematic representation of MIS. The Landau-level fan charts for two subbands with a parabolic dispersion and equal effective masses, with $E=E_i+\hbar\omega_c(n+1/2)$, $m^*=0.043m_0$, and the energy separation given by $E_{10}=31.2$ meV. Here m^* and E_{10} were chosen to be the same as in Fig. 6, where m^* is the effective mass for the $H1$ subband at E_F. The dotted lines show the particular magnetic fields where the two sets of Landau levels are completely aligned, and hence the intersubband scattering rate should be resonantly enhanced. The integers in the boxes are the ratios between E_{10} and $\hbar\omega_c$, i.e., $E_{10}=p\hbar\omega_c$.

TABLE I. Sample parameters.

Sample	d_w (nm)	Doping mode	μ ($10^4\ cm^2/V\ s$)	n_{Hall} ($10^{12}\ cm^{-2}$)	F_{H1-} (T)	F_{H1+} (T)	F_{E2} (T)	n_{SdH} ($10^{12}\ cm^{-2}$)
Q1484	20	Asym.	4.62	1.34	17.89	27.37	5.26	1.35
Q1545	20	Sym.	18.8	2.49	30.6		20.45	2.46

bands, in a perpendicular magnetic field and at a constant temperature can lead to an erroneous identification of the Rashba effect. Furthermore, according to the authors, a beating pattern due to MIS can manifest itself even in a one-subband 2DEG, because of thermal excitation[9] and Landau level broadening due to defects.[11]

Up until now most of the experimental studies on Rashba splitting have been devoted to semiconductor heterostructures with one occupied subband. Rowe *et al.*[11] studied a gated InAs/GaSb QW with two occupied subbands and found no Rashba splitting for both subbands over a wide carrier range from 4.8×10^{11} to $3.6\times10^{12}\ cm^{-2}$, however, MIS was observed. In contrast, Hu *et al.*[17] observed Rashba splitting in both subbands in an $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ heterojunction. For the II-VI narrow-gap system of HgTe QW's, we[18] recently reported a large Rashba splitting in the first conduction subband due to its heavy-hole nature and as expected an unresolved smaller splitting in the second subband.

It should be pointed out that the MIS model proposed by Raikh *et al.* is based on a simplified model that assumes a parabolic subband dispersion and equal effective masses for both subbands. The band nonparabolicity effect, the Zeeman spin splitting, and Rashba spin splitting were completely ignored. Because MIS is related to the resonant enhancement of the intersubband scattering rate due to the complete alignment of Landau levels of the two subbands, it should be influenced strongly by the factors mentioned above. But all the experimental investigations of MIS have been based on this simple band-structure model.

HgTe-based type-III heterostructures have aroused much interest due to their unique band structures.[21] An introduction to this system can be found in Ref. 18 and references therein. Pfeuffer-Jeschke *et al.*[22] reported values for the effective mass m^* for a series of QW's with the same well width of 9 nm, but different carrier concentration n_s. Here m^* increases from $0.016m_0$ at $1\times10^{11}\ cm^{-2}$ to $0.035m_0$ at $1\times10^{12}\ cm^{-2}$ due to the strong band nonparabolicity effect. The Zeeman spin splitting is relatively large, with an effective g factor of about 20 for a symmetric QW measured in a tilted magnetic field.[23] A large Rashba spin splitting in this system has recently been reported[18,24] for a QW with two occupied subbands. Therefore HgTe QW's provide the opportunity to study the influence of a complex band structure on the MIS effect and also the possible influence of MIS on Rashba spin splitting.

In order to study the MIS effect in HgTe QW's, the magnetoresistance of a symmetric and an asymmetric HgTe QW, both with two occupied subbands, was measured in the temperature range between 1.6 and 70 K. Theoretical calculations based on an 8×8 $\mathbf{k}\cdot\mathbf{p}$ model have also been carried out. Excellent agreement between experiment and theory has been achieved, which confirms the absence of the MIS effect in HgTe QW's. The Rashba spin splitting in HgTe QW's (Ref. 18) is free of the influence of the MIS effect.

II. EXPERIMENTAL AND THEORETICAL DETAILS

HgTe QW's were grown by molecular beam epitaxy (MBE) on $Cd_{0.96}Zn_{0.04}Te(001)$ substrates. The growth details have been published elsewhere.[25] After an approximately 60-nm-thick CdTe buffer, the QW structure was grown. The samples were modulation doped symmetrically or asymmetrically with iodine, on both or only one side of the HgTe layer, for samples Q1545 and Q1484, respectively. Both samples have the same well width of 20 nm. The doped $Hg_{0.32}Cd_{0.68}Te$ layer is separated from the HgTe layer by an 8-nm-thick $Hg_{0.32}Cd_{0.68}Te$ spacer. Finally, a 20-nm-thick CdTe cap layer was grown. The sample parameters are summarized in Table I. After growth, samples with Hall geometry were fabricated by standard photolithography. The magnetoresistance was measured using ac lock-in techniques in magnetic fields up to 10 T and at temperatures between 1.6 and 70 K. Care was taken in order to avoid electrical heating by the measuring current.

In order to compare with the measured longitudinal resistivity, ρ_{xx}, the oscillations of the density of states (DOS) in a magnetic field were calculated in the framework of an 8×8 $\mathbf{k}\cdot\mathbf{p}$ model.[26] The band-structure parameters employed in calculations of the Landau levels and DOS are listed in Table II. The details of the band-structure calculations are described elsewhere.[18,26] We have adopted the following relationship for the DOS of Landau levels in the lowest-order cumulant approximation (LOCA) approach according to Gerhardts:[27]

TABLE II. Band-structure parameters for HgTe and CdTe at $T=0$ K in calculations of Landau levels and the density of states.

	E_g (eV)	Δ (eV)	E_p (eV)	F	γ_1	γ_2	γ_3	κ	ϵ
HgTe	−0.303	1.08	18.8	0	4.1	0.5	1.3	−0.4	21
CdTe	1.606	0.91	18.8	−0.09	1.47	−0.28	0.03	−1.31	10.4

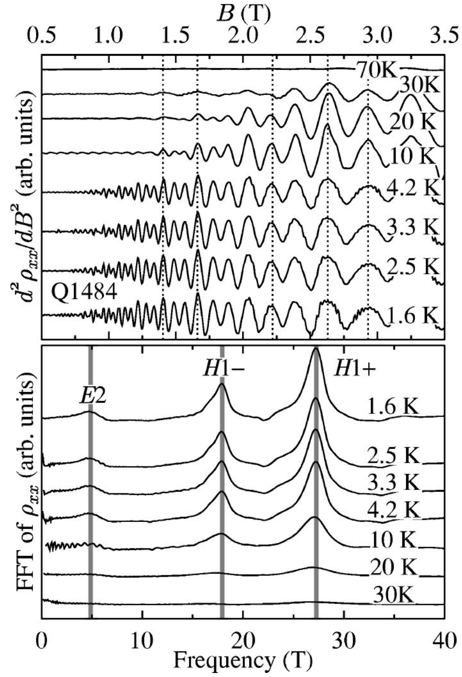

FIG. 2. The second derivative of ρ_{xx} (top panel) and the corresponding FFT (bottom panel) of an asymmetrically modulation doped *n*-type HgTe QW, Q1484, in the temperature range between 1.6 and 70 K. In the bottom panel, the subband notations are indicated. The dotted (top panel) and thick vertical lines (bottom panel) are merely guides to the eye.

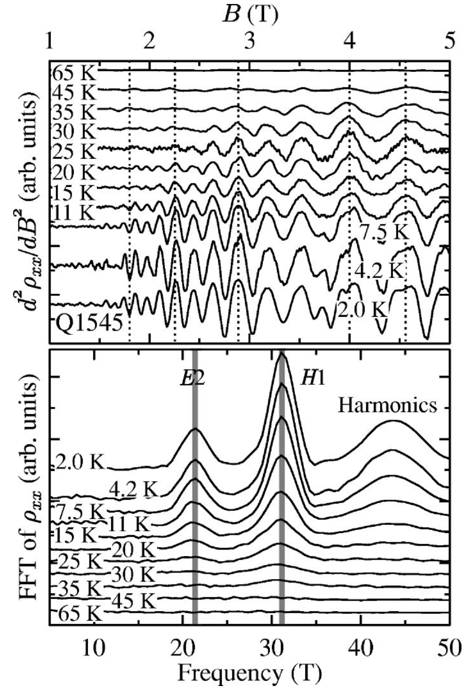

FIG. 3. The second derivative of ρ_{xx} (top panel) and the corresponding FFT (bottom panel) of a symmetrically modulation doped *n*-type HgTe QW, Q1545, in the temperature range between 2 and 65 K. In the bottom panel, the subband indices are also indicated. The dashed (top panel) and thick vertical lines (bottom panel) are merely guides to the eye.

$$D(E)=\frac{1}{2\pi l_c^2}\sum_n \frac{1}{\sqrt{\pi\Gamma^2}}\exp\left[-\frac{(E-E_n)^2}{\Gamma^2}\right], \tag{1}$$

where n is the Landau level index, $l_c=\sqrt{\hbar/eB}$ the magnetic length, $\Gamma=\Gamma_0\sqrt{B}$ the broadening of the Landau levels, and Γ_0 a constant. In the following the experimental SdH oscillations will be compared with the calculated DOS at E_F.

III. RESULTS AND DISCUSSION

A. Temperature dependence of SdH oscillations and their fast Fourier transform

In Figs. 2 and 3 are shown the SdH oscillations and their fast Fourier transform (FFT) at various temperatures, for an asymmetric and a symmetric QW, Q1484 and Q1545, respectively. For clarity, all the curves are shifted and some of them are multiplied by a factor. In order to completely eliminate the parabolic background, the second derivative of ρ_{xx} has been employed. With increasing temperature, the amplitude of the SdH oscillations and its envelope gradually damp out, but the phase of the peaks remains constant for both samples over the whole temperature range, as indicated in the top panels of Figs. 2 and 3. In contrast to the results for the $Al_{0.3}Ga_{0.7}As/GaAs$ heterojunction and the pseudomorphic $Al_{0.3}Ga_{0.7}As/In_{0.1}Ga_{0.9}As/GaAs$ QW investigated by Sander *et al.*,[28] where a phase change in the peaks of the magnetoresistance oscillations and their envelope was observed with increasing temperature, due to the different temperature dependences of SdH and MIS. This is obvious experimental evidence that MIS is absent in both symmetric and asymmetric HgTe QW's.

The self-consistently calculated band structure at zero magnetic field is very similar to that displayed in Fig. 3 of Ref. 18 and is omitted here. HgTe QW's with a well width larger than 6 nm have a so-called inverted band structure,[21] in which the $H1$ subband becomes the first conduction subband and the $E2$ subband is now the second conduction subband. $H1$ and $E2$ are the usual subband notation; $H1$ denotes the first heavy-hole subband and $E2$ the second conduction subband. The corresponding subband notations for the FFT peaks are indicated in the bottom panels of Figs. 2 and 3. Of the two occupied subbands, $E2$ is degenerate in both samples, however, the $H1$ subband is spin split (its two split states are labeled as $H1+$ and $H1-$) in the asymmetric sample, but degenerate in the symmetric one, as can be easily demonstrated from the charge carrier densities deduced from the SdH oscillations, n_{SdH}, and the Hall coefficient, n_{Hall}; the equivalence of these densities is fulfilled within experimental error if the multiplication factors for the F_{H1-} and F_{H1+} peaks are 1 for the former and that for the F_{H1} peak is 2 for the latter, i.e., $n_{\mathrm{Hall}}=(F_{H1+}+F_{H1-}+2F_{E2})e/h$ and $n_{\mathrm{Hall}}=(2F_{H1}+2F_{E2})e/h$, respectively. Here F_{H1+}, F_{H1-}, F_{H1}, and F_{E2} are the corresponding frequencies of the FFT peaks indicated in Figs. 2 and 3. The values of these frequencies, together with n_{SdH} and n_{Hall}, are listed in Table I. The conclusion that can be drawn from this very good agreement between n_{Hall} and n_{SdH} is that the peaks

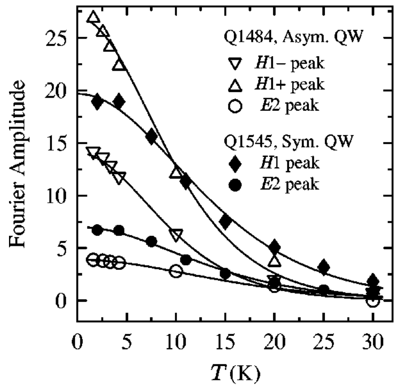

FIG. 4. Fourier amplitudes versus temperature for samples Q1484 and Q1545. Their temperature dependence can be accurately reproduced using $X/\sinh(X)$, as indicated by the solid lines.

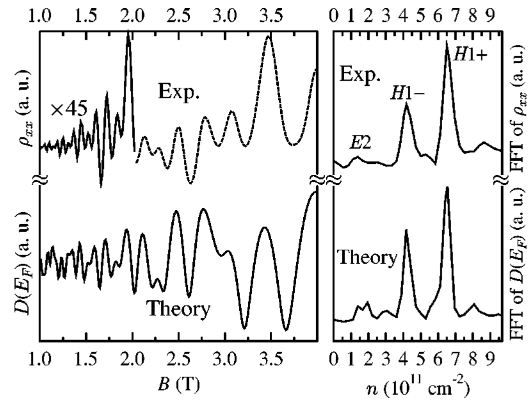

FIG. 5. The left panel shows a comparison between the experimental ρ_{xx} (upper curve) and the calculated density of states (DOS) at E_F in a magnetic field (lower curve) below 4 T. The right panel shows the corresponding FFT of ρ_{xx} (upper curve) and DOS (lower curve).

in the FFT of the SdH oscillations indeed represent the carrier densities in separate subbands and are not related to MIS, as have been observed in Ref. 11. This is clear experimental evidence of Rashba spin splitting in HgTe QW's. The strong Rashba spin splitting in the $H1$ subband and the unresolved splitting in the $E2$ subband are a consequence of the heavy-hole character of the $H1$ subband and the light-particle nature of the $E2$ subband, which is an admixture of the light-hole and electron states.[18]

The above conclusion can also be corroborated by the temperature variation of the FFT amplitudes shown in Fig. 4. In order to ensure a systematic comparison of the Fourier amplitudes, a FFT was performed over the same magnetic field range for all temperatures. The resulting variation can be accurately reproduced by the normal relationship for the temperature dependence of the amplitudes of SdH oscillations:[29]

$$A(T)=X/\sinh(X), \tag{2}$$

where $X=2\pi^2 k_B T/\hbar\omega_c$. Whereby, m^* is taken to be $0.043m_0$ and $0.044m_0$ for samples Q1484 and Q1545, respectively. This is a further proof that the FFT peaks labeled $H1$ and $E2$ in Figs. 2 and 3 are indeed related to SdH oscillations, and not to MIS, which has been shown to be temperature insensitive.[10,11]

B. Comparison with the calculated DOS and Landau levels

In Fig. 5 the experimental ρ_{xx} for the asymmetric sample is compared with the calculated DOS at E_F in the left panel, and their corresponding FFT's are shown in the right panel. In the theoretical calculations, Γ_0 in Eq. (1) has been taken to be 1.5 meV. And in order to get the best agreement with experiment, it has been assumed that 10% of the total electrons in the well do not come from the doped layer on the substrate side, but from the top undoped barrier. This is reasonable since the $Hg_{0.32}Cd_{0.68}Te$ spacer and barrier have an unknown degree of background doping. With this assumption, the positions of the extrema in ρ_{xx} can be very well reproduced by the theory, as shown in the left panel of Fig. 5. This clearly demonstrates that ρ_{xx} can be accurately reproduced by the summation of the DOS of two sets of Landau levels belonging to two different subbands. In other words, ρ_{xx} is entirely composed of SdH oscillations of two subbands over the whole temperature range. This completely rules out MIS oscillations. Another point to be noted is that one cannot expect the line shapes of ρ_{xx} and the calculated DOS to be in agreement, because localization effects in the band tails of the Landau levels have not been taken into account in the theoretical DOS calculation, which should have a pronounced influence on the amplitude of the experimental ρ_{xx}. The localization effect of the Landau levels in HgTe QW's is prominent, since the Hall resistivity ρ_{xy} shows partly developed quantum Hall plateaus at 1.6 K even at low magnetic fields down to 1.5 T for both samples.

From the FFT of ρ_{xx} and $D(E_F)$, shown in the right panel of Fig. 5, it can be seen that the peak positions of the $H1-$ and $H1+$ subbands show very good agreement between experiment and theory. And they also show very good agreement with the carrier densities deduced from the band-structure calculation at zero magnetic field (not shown here). This reflects the fact that Rashba spin splitting can be unambiguously deduced from the FFT of SdH oscillations in HgTe QW's, as a natural consequence of the absence of the MIS effect. This is in contrast to the conclusions of Rowe *et al.* for InAs/GaSb QW's,[11] that a mixing of MIS and SdH led to a beating pattern in the magnetoresistance, which could be falsely ascribed to Rashba spin splitting. The peak corresponding to the $E2$ subband shows a weak splitting in the theoretical calculation, but a negligible, albeit unresolved splitting in the experiment. This difference can be explained by the broadening of Landau levels, due to temperature and impurity scattering.

The reasons for the absence of MIS in HgTe QW's with an inverted band structure lie in their complex band structure and hence extremely irregular Landau-level alignment, as shown in Fig. 6, for the asymmetrical sample Q1484. Also shown in this figure is the oscillation of E_F. Compared with Fig. 1, strong band nonparabolicity is obvious from the nonlinear behavior of the Landau levels, especially for those corresponding to the $H1$ subband. The crossing of Landau levels of the $H1$ subband is caused by the large difference in

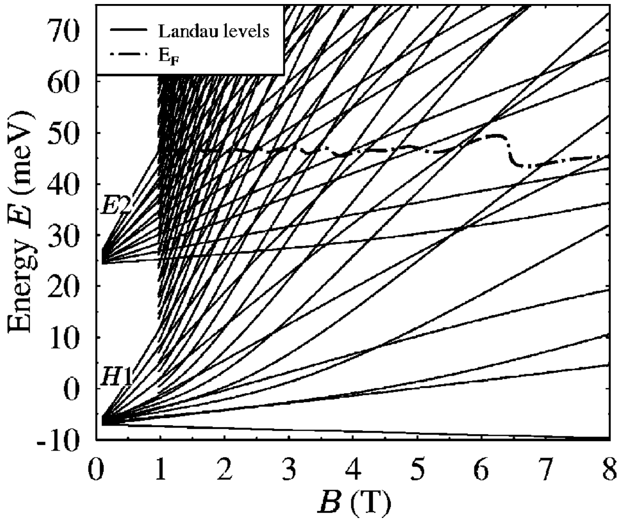

FIG. 6. The calculated Landau levels of the $H1$ and $E2$ subbands for sample Q1484. The Fermi energy E_F is shown by the dash-dotted line. E_F has been calculated by taking into account the broadening of the Landau levels, according to Eq. (1), with $\Gamma_0 = 1.5$ meV.

the dispersion of the two sets of Landau levels originating from the two strongly Rashba spin-split states at zero magnetic field. The Landau levels of the $E2$ subband are much more regular because of the much smaller Rashba splitting in this band.[18] The details of the Landau levels will not be discussed further: here, we are merely interested in the irregular alignment of the Landau levels, compared to the parabolic case shown in Fig. 1.

As discussed above, MIS comes from enhanced resonant intersubband scattering, due to the completely periodic alignment of the two sets of Landau levels belonging to two different subbands, as shown by the dotted lines in Fig. 1. A typical example of this case is a GaAs/GaAlAs heterostructure, whose first and second conduction subbands are nearly parabolic. The difference in the effective masses of the two conduction subbands will be less than 6% for a GaAs/AlGaAs QW with a well width of 5 nm.[30] But from the much more complex Landau levels of the HgTe QW's shown in Fig. 6, it can be seen first, that the magnetic field positions near E_F at which the Landau levels of $H1$ and $E2$ subbands are aligned are not periodic with $1/B$ as is the case in Fig. 1. Thus we cannot expect a peak related to MIS in the FFT of ρ_{xx} for HgTe QW's even though there may be appreciable intersubband scattering. Second, it is clear that at no particular magnetic fields can the Landau levels from different subbands be completely aligned in HgTe QW's, as indicated by the dotted lines in Fig. 1 for the parabolic case. Therefore, it is reasonable to conclude that the intersubband scattering rate at resonant magnetic fields in HgTe QW's cannot be enhanced to a comparable degree as in the parabolic case of Fig. 1. The complex Landau-level alignment in HgTe QW's suppresses magneto-intersubband scattering.

IV. CONCLUSION

Magneto-intersubband scattering, which is a general feature in some III-V heterostructures with two occupied subbands, has been demonstrated to be absent in both experimental results and theoretical calculations for HgTe QW's. This has been ascribed to the irregular Landau-level alignment in HgTe QW's, which suppresses the intersubband scattering rate. Consequently, Rashba spin splitting can be properly identified from the experimental magnetoresistance in a perpendicular magnetic field and at a constant temperature.

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