Electron spin relaxation in p-type GaAs quantum wells

Y Zhou\(^1\), J H Jiang\(^2\) and M W Wu\(^{1,2,3}\)

\(^1\) Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, Anhui 230026, People’s Republic of China

\(^2\) Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, People’s Republic of China

E-mail: mwwu@ustc.edu.cn.

New Journal of Physics 11 (2009) 113039 (16pp)
Received 8 July 2009
Published 20 November 2009
Online at http://www.njp.org/
doi:10.1088/1367-2630/11/11/113039

Abstract. We investigate electron spin relaxation in p-type GaAs quantum wells from a fully microscopic kinetic spin Bloch equation approach, with all the relevant scatterings, such as electron–impurity, electron–phonon, electron–electron Coulomb, electron–hole Coulomb and electron–hole exchange (the Bir–Aronov–Pikus (BAP) mechanism) scatterings, explicitly included. Via this approach, we examine the relative importance of the D’yakonov–Perel’ (DP) and BAP mechanisms in wide ranges of temperature, hole density, excitation density and impurity density, and present a phase-diagram-like picture showing the parameter regime where the DP or BAP mechanism is more important. It is discovered that in the impurity-free case the temperature regime where the BAP mechanism is more efficient than the DP one is around the hole Fermi temperature for high hole density, regardless of excitation density. However, in the high impurity density case with the impurity density identical to the hole density, this regime is roughly from the electron Fermi temperature to the hole Fermi temperature. Moreover, we predict that for the impurity-free case, in the regime where the DP mechanism dominates the spin relaxation at all temperatures, the temperature dependence of the spin relaxation time (SRT) presents a peak around the hole Fermi temperature, which originates from the electron–hole Coulomb scattering. We also predict that at low temperature, the

\(^3\) Author to whom any correspondence should be addressed.
hole-density dependence of the electron SRT exhibits a *double-peak* structure in the impurity-free case, whereas it shows first a peak and then a valley in the case of identical impurity and hole densities. These intriguing behaviors are due to the contribution from holes in high subbands.

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### 1. Introduction

In recent years, much attention has been devoted to semiconductor spintronics both theoretically and experimentally due to the potential application of spin-based devices [1]–[3]. In order to manipulate the spin relaxation such that the information is well preserved before required operations are completed, it is crucial to gain a thorough understanding of spin relaxations. In p-doped III–V semiconductors, the main electron spin relaxation mechanisms have been recognized as [1] the Bir–Aronov–Pikus (BAP) mechanism [4] and the D’yakonov–Perel’ (DP) mechanism [5]. In the DP mechanism, electron spins decay due to their precessions around the momentum-dependent spin–orbit fields (inhomogeneous broadening) [6] during the free flight between adjacent scattering events. In the BAP mechanism, spin relaxes due to spin flip caused by exchange interaction with holes. It was believed that in p-doped bulk samples, the BAP mechanism dominates the spin relaxation process at high doping density and low temperature, whereas the DP mechanism is more important at low doping density and high temperature [1], [7]–[10]. In a two-dimensional system, Maialle [11] calculated the spin relaxation time (SRT) due to these two mechanisms at zero temperature using the single-particle approach and showed that these two SRTs have nearly the same order of magnitude. However, as pointed out by Zhou and Wu recently [12], there are some common problems in the published literature: the SRT due to the BAP mechanism was calculated based on the elastic scattering approximation, which is invalid at low temperature due to the omission of Pauli blocking. Also, the investigation of the SRT due to the DP mechanism was also inadequate because the Coulomb scattering is not included in the framework of single-particle theory.

Zhou and Wu applied the fully microscopic kinetic spin Bloch equation (KSBE) approach [6, 13] to investigate the spin relaxation in p-type GaAs quantum wells [12]. The KSBE approach has achieved good success in the study of spin dynamics in semiconductors, where not only the results are in good agreement with the previous experiments, but also many predictions have been confirmed by the latest experiments [6], [12]–[30]. Via this approach, they explicitly included all the relevant scatterings and obtained the accurate SRT due to these
two mechanisms. It was found that the BAP mechanism is always less efficient than the DP mechanism for moderate and high excitation densities where $N_{ex} \gtrsim 0.1N_h$ ($N_{ex}$ ($N_h$) is the excitation (hole) density), in contrast to the common belief in the literature [1], [7]–[10]. This claim has very recently been confirmed experimentally by Yang et al [29]. A similar conclusion was also obtained in bulk GaAs later [19].

However, for very low excitation density where the Pauli blocking of electrons is negligible, for high hole density where the contribution from the high subbands or different hole bands becomes significant and/or for high impurity density where the spin relaxation due to the DP mechanism is suppressed, whether the BAP mechanism can be more efficient is still questionable. In the present work, we extend the KBSEs to include both the lowest subband of light hole (LH) and the lowest two subbands of heavy hole (HH), and compare the relative importance of the DP and BAP mechanisms in wider ranges of temperature, hole density, excitation density and impurity density. We present a ‘phase-diagram-like’ picture indicating the dominant spin relaxation mechanism. In the case with no impurity and high excitation density, our results show that the BAP mechanism is unimportant at low temperature, in agreement with [12]. Nevertheless, since more hole subbands and bands are included in our model, we are able to discuss the case with higher hole density. We find that the BAP mechanism can surpass the DP mechanism at high temperature for sufficiently high hole density. In the case with no impurity and low excitation density, the BAP mechanism can surpass the DP mechanism for wider hole density and temperature ranges. Moreover, we also find that in both cases above, the regime where the BAP mechanism is more efficient is always around the hole Fermi temperature for high hole density, regardless of excitation density. However, in the high impurity density case with the impurity density being identical to the hole density, the behavior is very different from the impurity-free case: the regime of hole density where the BAP mechanism is more efficient becomes larger, and the regime of temperature becomes wider, ranging roughly from the electron Fermi temperature to the hole Fermi temperature. We also show that the multi-hole-subband effect leads to a very intriguing hole-density dependence of SRT at low temperature.

This paper is organized as follows. In section 2, we set up the KSBEs. In section 3, we compare the relative importance of the BAP and DP mechanisms in different parameter regimes and investigate the multi-hole-subband effect. We conclude in section 4. A comparison of the calculation from the KSBEs with the experimental data of a p-type GaAs quantum well is given in the appendix.

2. Kinetic spin Bloch equations

We investigate a p-type (001) GaAs quantum well of width $a$ with its growth direction along the $z$-axis. The width is assumed to be small enough so that only the lowest subband of electron, the lowest two subbands of HH and the lowest subband of LH are relevant for the electron and hole densities we discuss. The envelope functions of the relevant subbands are calculated under the finite-well-depth assumption [12, 17]. The barrier layer is chosen to be Al$_{0.4}$Ga$_{0.6}$As where the barrier heights of electron and hole are 328 and 177meV, respectively [31]. We focus on the metallic regime where most of the carriers are in extended states. Since the hole spins relax very rapidly (only several picoseconds), we assume that the hole system is always in equilibrium.

Via the nonequilibrium Green function method [32], we construct the KSBEs as follows [12, 13]:

$$\partial_t \hat{\rho}_k = \partial_t \hat{\rho}_k |_{coh} + \partial_t \hat{\rho}_k |_{scat}$$

(1)
with $\hat{\rho}_k$ representing the electron single-particle density matrix with a two-dimensional momentum $k = (k_x, k_y)$, whose diagonal and off-diagonal elements describe the electron distribution function and spin coherence, respectively. The coherent term can be written as ($\hbar = 1$ throughout this paper)

$$\partial_t \hat{\rho}_k |_{coh} = -i \left[ \mathbf{h}(k) \cdot \hat{\sigma} + \hat{\Sigma}_{HF}(k), \hat{\rho}_k \right],$$

(2)
in which $[A, B] \equiv AB - BA$ is the commutator. $\mathbf{h}(k)$ represents the spin–orbit coupling of electrons composed of the Dresselhaus [33] and Rashba [34] terms. For GaAs quantum wells, the Dresselhaus term is dominant [35] and

$$\mathbf{h}(k) = 2\gamma_D \left( k_x (k_y^2 - \langle k_y^2 \rangle), k_y (\langle k_y^2 \rangle - k_x^2), 0 \right),$$

(3)
where $\langle k_y^2 \rangle$ stands for the average of the operator $-(\partial/\partial z)^2$ over the state of the lowest subband of electron, and $\gamma_D = 8.6 \text{ eV} \text{ Å}^3$ denotes the Dresselhaus spin–orbit coupling coefficient [25, 36]. $\hat{\Sigma}_{HF}(k)$ is the effective magnetic field from the Coulomb Hartree–Fock contribution [14]. For the screened Coulomb potential, the screening from electrons and holes is calculated under the random phase approximation [12, 37]. The scattering term $\partial_t \hat{\rho}_k |_{scat}$ consists of electron–impurity, electron–phonon, electron–electron Coulomb, electron–hole Coulomb and electron–hole exchange scatterings. The expressions of these scatterings are given in detail in [12]. Here we just extend the electron–hole Coulomb and exchange scatterings to the multi-hole-subband case. The expression of electron–hole Coulomb scattering is similar to that in [12]. The complete electron–hole exchange scattering term is written as

$$\partial_t \hat{\rho}_k |_{BAP} = -\pi \sum_{k', q, \lambda, \lambda'} \delta (\epsilon_{k'q} - \epsilon_k + \epsilon^h_{k'q\lambda} - \epsilon^h_{k'q,-\lambda'}) |T^{\eta}_{\lambda\lambda'}(k + k' - q)|^2 \left[ \hat{\delta}_{\eta} \hat{\rho}_{k'q\lambda} \hat{\delta}_{-\eta} \hat{\rho}_{k'q,-\lambda'} \right] \times (1 - f^h_{k'\lambda'}) f^h_{k'q\lambda'} - \hat{\delta}_{\eta} \hat{\rho}_{k'q\lambda} \hat{\delta}_{-\eta} \hat{\rho}_{k'q,-\lambda'} f^h_{k'\lambda'} (1 - f^h_{k'q,-\lambda'}) \right] + \text{h.c.}$$

(4)

Here $\hat{\rho}_k^c = 1 - \hat{\rho}_k$ and $\hat{\rho}_k^c = \hat{\rho}_k$ are the electron density matrices; $\hat{\delta}_\pm = \hat{\delta}_x \pm i \hat{\delta}_y$ are the electron spin ladder operators. $\lambda = HH(a), LH(a)$ with the superscript being the subband index of hole. $f^h_{k\lambda}$ is the hole distribution on the $\lambda$th hole band. The matrix $\hat{T}^\pm$ comes from the long-range term of the electron–hole exchange interaction Hamiltonian and can be written as $\hat{T}^\pm = \frac{3}{8} \Delta E_{LT} \hat{M}^\pm$ [38], where $\Delta E_{LT}$ is the longitudinal–transverse splitting in bulk, $|\phi_{3D}(0)|^2 = 1/(\pi a^3_0)$ with $a_0$ being the exciton Bohr radius, and $\hat{M}^-$ and $\hat{M}^+$ ($= (\hat{M}^-)^\dagger$) are operators in hole spin space. The matrix $\hat{M}^-$ is given by [38] (in the order of $|\frac{3}{2} \rangle \langle \frac{1}{2} |, | -\frac{3}{2} \rangle \langle \frac{1}{2} |, | \frac{3}{2} \rangle \langle \frac{3}{2} |, | -\frac{3}{2} \rangle \langle \frac{3}{2} |, | \frac{1}{2} \rangle \langle \frac{1}{2} |, | -\frac{1}{2} \rangle \langle \frac{1}{2} |)$

$$\hat{M}^- (K) = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & -F^0_{1111} K^2 + \frac{\sqrt{3}}{3} F^0_{1111} K^2 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & F^0_{1111} K^2 & 0 & -2 F^0_{1111} K^2 & 0 \\
0 & 0 & 0 & 0 & 0 & -F^0_{1111} K^2 \\
0 & 0 & 2 F^0_{1111} K^2 & 0 & 0 & 0 \\
0 & 0 & 0 & -4 F^0_{1111} K^2 & 0 & 0
\end{bmatrix},$$

(5)

$^4$ The contribution from the short-range term is negligible [19].

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Table 1. Material parameters used in the calculation.

| Parameter  | Value                      |
|------------|----------------------------|
| $g_e$      | $-0.44$                    |
| $m_e^{\perp}$ | $0.112 m_0$              |
| $m_e^{\parallel}$ | $0.067 m_0$             |
| $m_{HH}^{\perp}$ | $0.211 m_0$              |
| $m_{HH}^{\parallel}$ | $0.091 m_0$             |
| $\kappa_0$ | $12.9$                    |
| $\kappa_\infty$ | $10.8$                 |
| $D$        | $5.31 \times 10^3$ kg m$^{-3}$ |
| $v_{sd}$   | $2.48 \times 10^3$ m s$^{-1}$ |
| $\Xi$      | $8.5$ eV                  |
| $\Delta_{SO}$ | $0.341$ eV                |
| $\Delta E_{LT}$ | $0.08$ meV              |

where $\mathbf{K} = \mathbf{k} + \mathbf{k}' - \mathbf{q}$ is the center-of-mass momentum of the electron–hole pair with $K_\pm = K_x \pm i K_y$. The form factors can be written as

$$F_{\lambda\lambda'}^p (K) = \int \frac{dq_z}{2\pi} \frac{q_z^p}{K^2 + q_z^2} f_{\lambda\lambda'}(q_z)$$

with

$$f_{\lambda\lambda'}(q_z) = \int dz dz' \xi_\epsilon(z') \xi_\epsilon^*(z') e^{i q_z(z' - z)} \xi_\epsilon(z) \xi_\epsilon^*(z).$$

In equation (5), it is seen that most of the nonzero elements in matrix $\hat{M}$ contain $K_\pm^2$ or $K_\pm$, and thus the magnitudes of these terms increase with increasing $K$. The only exception is $M_{-1/2,1/2}^{-1}$, where the $K$ dependence is only from the form factor $F_{111}^0$. Consequently, the magnitude of $M_{-1/2,1/2}^{-1}$ decreases with $K$. This $K$ dependence contributes to an intriguing hole-density dependence of spin relaxation to be addressed in this work.

3. Results and discussions

By numerically solving the KSBEs with all the scatterings explicitly included, one is able to obtain the SRT from the temporal evolution of the electron spin polarization along the $z$-axis. We choose initial spin polarization $P = 4\%$ and well width $a = 10$ nm; the external magnetic field $B = 0$ unless otherwise specified. The other material parameters are listed in table 1.

3.1. Comparison of the BAP and DP mechanisms

We first examine the relative importance of the BAP and DP mechanisms for different parameters in p-type GaAs quantum wells. In figure 1, the ratio of the SRT due to the BAP mechanism to that due to the DP mechanism is plotted as a function of temperature and hole density in the cases with no/high impurity and low/high excitation densities. From this figure, one can recognize the parameter regime where the DP or BAP mechanism is more important. It is also shown that the multi-hole-subband effect becomes significant for high temperature and/or high hole density (the regime above the yellow solid curve). Here and hereafter, the model calculations are not sensitive to the initial spin polarization when it is small.
Figure 1. Ratio of the SRT due to the BAP mechanism to that due to the DP mechanism, $\tau_{\text{BAP}}/\tau_{\text{DP}}$, as a function of temperature and hole density with (a) $N_i = 0$, $N_{\text{ex}} = 10^{11}$ cm$^{-2}$; (b) $N_i = 0$, $N_{\text{ex}} = 10^9$ cm$^{-2}$; (c) $N_i = N_h$, $N_{\text{ex}} = 10^{11}$ cm$^{-2}$; and (d) $N_i = N_h$, $N_{\text{ex}} = 10^9$ cm$^{-2}$. The black dashed curves indicate the cases satisfying $\tau_{\text{BAP}}/\tau_{\text{DP}} = 1$. Note that the smaller the ratio $\tau_{\text{BAP}}/\tau_{\text{DP}}$ the more important the BAP mechanism. The yellow solid curves indicate the cases satisfying $\partial_{\mu h}[N_{LH,1} + N_{HH,2}]/\partial_{\mu h}N_h = 0.1$. In the regime above the yellow curve, the multi-hole-subband effect becomes significant.

multi-hole-subband refers to either the high HH subband or the LH subband. Although the multi-hole-subband effect has an important effect on electron spin relaxation in the relevant regime, the main physics is still the same as that in the single-hole-subband model. Therefore, in this subsection, we first discuss the general behavior about how the relative importance of the BAP and DP mechanisms is influenced by the temperature, hole density, excitation density and impurity density, which is analogous in both the multi-hole-subband and single-hole-subband models. We then investigate the special features from the contribution of high hole subbands in the next subsection.

In the case with no impurity and high excitation density (figure 1(a)), our results are consistent with [12]: the BAP mechanism is unimportant at low temperature, which is in stark contrast with the common belief in the literature [1], [7]–[10]. Moreover, since we extend the scope of our investigation to higher hole density by including more hole subbands in our model, it is discovered that the BAP mechanism can surpass the DP mechanism in the regime with high temperature and sufficiently high hole density (the regime embraced by the black dashed curve).

In the case with no impurity and low excitation density (figure 1(b)), one can see that the regime where the BAP mechanism surpasses the DP mechanism becomes larger. The underlying physics is shown in figure 2(a). It is seen that the SRTs due to the BAP and DP mechanisms both decrease with increasing excitation density ($N_{\text{ex}} = N_e$), but the amplitude of the latter is much
Figure 2. SRTs due to the DP and BAP mechanisms, the total SRT together with the ratio \( \tau_{\text{BAP}} / \tau_{\text{DP}} \) versus temperature \( T \) for \( N_{\text{ex}} = 10^9 \text{ cm}^{-2} \) (curves with •), \( 3 \times 10^{10} \text{ cm}^{-2} \) (curves with ▲) and \( 10^{11} \text{ cm}^{-2} \) (curves with ■) with hole-density \( N_h = 5 \times 10^{11} \text{ cm}^{-2} \) and impurity densities (a) \( N_i = 0 \) and (b) \( N_i = N_h \). The electron Fermi temperatures for those excitation densities are \( T_e^F = 0.41, 12.4 \) and \( 41.5 \text{ K} \), respectively. The hole Fermi temperature is \( T_h^F = 124 \text{ K} \). Note that the scale of \( \tau_{\text{BAP}} / \tau_{\text{DP}} \) is on the right-hand side of the frame. The multi-hole-subband effect is taken into account in the calculation.

The decrease of \( \tau_{\text{DP}} \) comes from the increase of the inhomogeneous broadening \( \langle |h_k|^2 \rangle \propto N_{\text{ex}} \) [14], and the decrease of \( \tau_{\text{BAP}} \) is mainly from the increase of the average electron velocity \( \langle v_k \rangle \propto N_{\text{ex}}^{0.5} \) [11]. Moreover, the increase of the Pauli blocking of electrons can partially compensate the effect of the increase of \( \langle v_k \rangle \) [12]. Consequently, \( \tau_{\text{BAP}} \) decreases with \( N_{\text{ex}} \) much more slowly than \( \tau_{\text{DP}} \) and the relative importance of \( \tau_{\text{BAP}} \) is enhanced for lower excitation density. It is also noted that when the electron system is in the nondegenerate regime \( (T > T_e^F = E_e^F/k_B) \), the inhomogeneous broadening and \( \langle v_k \rangle \) are not sensitive to \( N_{\text{ex}} \). Thus the ratio \( \tau_{\text{BAP}} / \tau_{\text{DP}} \) changes little with the excitation density.

Most cases we discuss in this paper are in the strong scattering regime, where \( \tau_{\text{DP}} \) increases with momentum scattering strength and decreases with inhomogeneous broadening.

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By comparing figures 1(a) and (b), it is seen that the regimes where the BAP mechanism is more efficient in both cases are around the hole Fermi temperature $T_F^h = E_F^h/k_B$ for high hole density. Here $E_F^h$ represents the Fermi energy of the hole at zero temperature, calculated with the HH$^{(1)}$, LH$^{(1)}$ and HH$^{(2)}$ subbands included. A typical case is shown in figure 2(a) for $N_h = 5 \times 10^{11}$ cm$^{-2}$. It is shown that the ratio $\tau_{\text{BAP}}/\tau_{\text{DP}}$ first decreases and then increases with increasing $T$. The minimum is around $T_F^h = 124$ K, regardless of excitation density. The underlying physics is as follows. On the one hand, the SRT due to the DP mechanism first increases and then decreases with $T$ and the peak appears around the hole Fermi temperature. This is because the electron–hole Coulomb scattering, which dominates the momentum scattering, increases with increasing temperature in the degenerate regime ($T < T_F^h$) and decreases with $T$ in the nondegenerate regime ($T > T_F^h$), similar to the electron–electron Coulomb scattering [17, 41, 42]. On the other hand, the SRT due to the BAP mechanism first decreases rapidly and then slowly with $T$. The decrease of $\tau_{\text{BAP}}$ is mainly from the decrease of the Pauli blocking of holes and the increase of the matrix elements in equation (5) [12]. In the high-temperature (nondegenerate) regime, Pauli blocking becomes very weak, and thus $\tau_{\text{BAP}}$ decreases slowly with $T$. Under the combined effect of these two mechanisms, a valley in the ratio $\tau_{\text{BAP}}/\tau_{\text{DP}}$ appears around $T_F^h$.

Moreover, we also show that in the regime where the DP mechanism is dominant at all temperatures, e.g. the high excitation density case (the curves with squares in figure 2(a)), the total SRT shows a peak around the hole Fermi temperature. This temperature dependence is similar to the peak first predicted theoretically and then confirmed experimentally in n-type samples [17, 21, 43]. The only difference is that the peak in the previous work comes from the electron–electron Coulomb scattering and hence appears around the electron Fermi temperature, whereas the peak here originates from the electron–hole Coulomb scattering and thus appears around the hole Fermi temperature.

Then we turn to the case of high impurity density with $N_i = N_h$ (figures 1(c) and (d)). In this case, the regime where the BAP mechanism is more important becomes larger than that in the impurity-free case. The scenario is that the higher impurity density strengthens the electron–impurity scattering and suppresses the DP mechanism, consequently enhancing the relative importance of the BAP mechanism. Interestingly, it is also seen that the temperature regime where the BAP mechanism surpasses the DP mechanism in this case is very different from that in the impurity-free case. This regime is roughly from the electron Fermi temperature to the hole Fermi temperature for high hole density. To explore the underlying physics, we plot the SRTs due to the BAP and DP mechanisms in figure 2(b) for $N_h = 5 \times 10^{11}$ cm$^{-2}$. It is seen that the SRT due to the DP mechanism first decreases slowly and then rapidly with temperature. This is because the electron–impurity scattering, which dominates the momentum scattering, has a very weak temperature dependence. Thus the temperature dependence of $\tau_{\text{DP}}$ is mainly determined by the inhomogeneous broadening from the spin–orbit coupling. It is also noted that the inhomogeneous broadening changes little with temperature when $T < T_F^e$, hence $\tau_{\text{DP}}$ varies with $T$ very mildly at low temperature. In contrast, as mentioned above, the SRT due to the BAP mechanism first decreases rapidly and then slowly with temperature. As a result, the temperature

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7 The hole-density $N_h$ consists of both holes from acceptors and those from optical excitation.

8 It is seen that in the case with $N_{ex} = 10^{11}$ cm$^{-2}$, the variation of the SRT due to the DP mechanism becomes very mild when $T < 10$ K. This is because this case belongs to the intermediate scattering regime, where $\tau_{\text{DP}}$ has a weak dependence on the scattering strength.
dependence of $\tau_{\text{BAP}}/\tau_{\text{DP}}$ can be easily understood. When $T < T^e_F$, $\tau_{\text{DP}}$ decreases with $T$ slower than $\tau_{\text{BAP}}$, thus the ratio decreases with $T$. In the case with $T > T^h_F$, $\tau_{\text{DP}}$ decreases with $T$ faster than $\tau_{\text{BAP}}$; hence the ratio increases with $T$. The ratio $\tau_{\text{BAP}}/\tau_{\text{DP}}$ varies mildly when temperature varies from $T^e_F$ to $T^h_F$. Consequently, when hole density is high enough, the BAP mechanism can surpass the DP mechanism in the temperature regime between these two temperatures. In particular, in the case with high impurity and very low electron excitation densities (figure 1(d)), the electron Fermi temperature (0.41 K) is much lower than the lowest temperature (5 K) of our computation and the hole Fermi temperature is close to the highest temperature (300 K) of our computation. As a result, the BAP mechanism dominates the spin relaxation in the whole temperature regime of our investigation.

We stress that the different behaviors in the impurity-free and high impurity density cases originate from the different dominant momentum scatterings: the electron–hole Coulomb scattering in the impurity-free case and the electron–impurity scattering in the high impurity density case. The different dominant scatterings lead to the different temperature dependences of $\tau_{\text{DP}}$, and hence the different behaviors of the $\tau_{\text{BAP}}/\tau_{\text{DP}}$ ratio. In the case with moderate impurity density, these two scatterings contribute to the DP spin relaxation, thus the trend of the temperature dependence of $\tau_{\text{DP}}$ is between those in the impurity-free and high impurity density cases. As a result, the temperature regime where the BAP mechanism is more efficient than the DP mechanism is from some temperature between the electron and hole Fermi temperatures.

3.2. Multi-hole-subband effect

Now we investigate the multi-hole-subband effect on spin relaxation. In our model, besides the first HH subband, we also consider the contribution from the first LH subband and the second HH subband. Since only the hole states around the Fermi surface can contribute to the electron–hole Coulomb or exchange scattering, we choose $\partial_{\mu h} N_{\lambda} / \partial_{\mu h} N_h$ as the criterion of the contribution from the $\lambda$ hole subband. We further show the regime where the contribution from high hole subbands becomes significant in figure 1 (the regime above the yellow curve), where $\partial_{\mu h} (N_{\text{LH}(1)} + N_{\text{HH}(2)}) / \partial_{\mu h} N_h > 0.1$. It is noted that we only discuss the combined effect of the DP spin relaxation from the LH(1) and HH(2) subbands in the following, as the effects on the electron–hole Coulomb scattering from these two subbands are analogous. Moreover, the matrix elements in equation (5) relevant to the HH(2) subband are one order of magnitude smaller than those relevant to the LH(1) subband for the relevant range of center-of-mass momentum $K$ in the following cases. Therefore, we only discuss the effect on the BAP spin relaxation from the LH(1) subband.

We first show how the multi-hole-subband effect influences the temperature dependence of spin relaxation. SRTs due to the DP and BAP mechanisms as well as the $\tau_{\text{BAP}}/\tau_{\text{DP}}$ ratio are plotted in figure 3 as a function of temperature for a typical case with $N_i = 0$, $N_h = 5 \times 10^{11} \text{cm}^{-2}$ and $N_{\text{ex}} = 10^{11} \text{cm}^{-2}$. It is seen that after considering the contribution from high hole subbands, $\tau_{\text{BAP}}$ decreases but $\tau_{\text{DP}}$ increases, and hence the importance of the BAP mechanism is enhanced. The underlying physics is as follows. The states in high hole subbands provide an additional scattering channel, and the electron–hole Coulomb and exchange scatterings are both enhanced. The former suppresses the DP mechanism in the strong scattering limit, and the latter leads to an enhancement of the BAP mechanism. Both make the BAP mechanism become more important compared with the DP mechanism. It is also seen that the multi-hole-subband effect.
Figure 3. SRTs due to the DP and BAP mechanisms, the total SRT together with the ratio $\tau_{\text{BAP}}/\tau_{\text{DP}}$ versus temperature $T$ with $N_i = 0$, $N_h = 5 \times 10^{11} \text{cm}^{-2}$ and $N_{ex} = 10^{11} \text{cm}^{-2}$. The hole and electron Fermi temperatures are $T_F^h = 124$ K and $T_F^e = 41$ K, respectively. The solid curves are the results calculated with the lowest two subbands of HH and the lowest subband of LH. The dashed curves are those from only the lowest subband of HH. Note that the scale of $\tau_{\text{BAP}}/\tau_{\text{DP}}$ is on the right-hand side of the frame.

becomes more pronounced at high temperature. This is because the occupation of the high hole subbands becomes larger when temperature increases.

From figure 3, one also finds that the multi-hole-subband effect does not significantly affect the trend of the temperature dependence of the SRT. The main change after the inclusion of the high hole subbands is that the temperature at which $\tau_{\text{BAP}}/\tau_{\text{DP}}$ reaches a minimum becomes closer to the hole Fermi temperature. The underlying physics is as follows. In the degenerate regime ($T < T_F^h$), it is seen that compared with those in the single-hole-subband model, $\tau_{\text{DP}}$ ($\tau_{\text{BAP}}$) in the multi-hole-subband model increases (decreases) faster with increasing temperature, both originate from the increase in the occupation of the high hole subbands and hence the increase of the electron–hole Coulomb and exchange scatterings. This leads to a faster decrease of $\tau_{\text{BAP}}/\tau_{\text{DP}}$ with increasing temperature when $T < T_F^h$ [19, 20]. Nevertheless, in the nondegenerate regime ($T > T_F^h$), it is seen that $\tau_{\text{DP}}$ ($\tau_{\text{BAP}}$) in the multi-hole-subband model decreases faster (slower) than that in the single-hole-subband model. The acceleration in the decrease of $\tau_{\text{DP}}$ can be understood as follows. In the nondegenerate regime, the electron–hole Coulomb scattering decreases with temperature. With the contribution from high hole subbands, the electron–hole Coulomb scattering becomes stronger and thus the decrease rate also becomes larger. Therefore, $\tau_{\text{DP}}$ decreases faster in the multi-hole-subband calculation [19, 20]. The slowdown in the decrease of $\tau_{\text{BAP}}$ originates from the anomalous $K$ dependence of the matrix element $M_{-1/2,1/2}^-$ in equation (5), which is relevant to the LH(1) subband. As discussed above, in the nondegenerate regime, the temperature dependence of $\tau_{\text{BAP}}$ is mainly from the matrix elements. It is also noted that the magnitude of $M_{-1/2,1/2}^-$ decreases with $K$, whereas the magnitudes of the other matrix elements increase with $K$. With the increase of temperature, more holes and electrons are distributed at larger momentums, the contribution from $M_{-1/2,1/2}^-$ decreases and the
contributions from the other matrix elements increase. These two trends counteract with each other and make τ_{BAP} decrease with increasing T very slowly at high temperature. Consequently, when \( T > T_F^b \), the ratio \( \tau_{BAP}/\tau_{DP} \) shows a steeper increase with rising temperature in the multi-hole-subband calculation. Therefore, both trends when the temperature is below and above \( T_F^b \) make the minimum of \( \tau_{BAP}/\tau_{DP} \) appear at the temperature closer to \( T_F^b \) in the multi-hole-subband calculation.

We also investigate the multi-hole-subband effect on the hole-density dependence of spin relaxation. In figure 4, SRTs due to various mechanisms, the total SRT together with the ratio \( \tau_{BAP}/\tau_{DP} \) are plotted as a function of hole density. It is interesting to see from figure 4(a) that at
low temperature, spin relaxation has a very intriguing hole-density dependence. In the impurity-free case, the hole-density dependence of the total SRT shows a double-peak structure, i.e. it first increases slightly, then decreases, again increases rapidly and finally decreases with increasing hole density. In the high impurity density case with \( N_i = N_h \), the total SRT shows first a peak and then a valley as a function of hole density. We first discuss the impurity-free case, where the BAP mechanism is negligible and the double-peak structure is solely from the DP mechanism. The first peak can be understood as follows. The electron–hole Coulomb scattering increases with \( N_h \) in the nondegenerate regime \( (E_F^h < k_B T) \) from the increase of hole distribution, but decreases with \( N_h \) in the degenerate regime \( (E_F^h > k_B T) \) due to the increase of the Pauli blocking of holes \([19, 20]\). Hence \( \tau_{DP} \) first increases and then decreases with \( N_h \), with the peak appearing around the hole density satisfying \( E_F^h = k_B T \). This behavior is similar to the peak predicted in n-type samples \([19]\), where the peak originates from the electron–electron Coulomb scattering and hence appears around the electron density satisfying \( E_F^e = k_B T \). It is also seen that the second peak only appears in the multi-hole-subband calculation, but is absent in the single-hole-subband calculation (the green dashed curve with circles), which indicates that this peak comes from the contribution of the electron–hole Coulomb scattering from high hole subbands.

In fact, the scenario is similar to the first one. When \( N_h > 6 \times 10^{11} \, \text{cm}^{-2} \), the contribution from the LH\(^{(1)}\) subband becomes important.\(^9\) Since the holes in the LH\(^{(1)}\) subband are still in the nondegenerate regime, the electron–hole Coulomb scattering increases with increasing hole density. Thus \( \tau_{DP} \) increases with \( N_h \). When \( N_h > 9 \times 10^{11} \, \text{cm}^{-2} \), i.e. \( E_F^h - \Delta E_{\text{LH}} = k_B T \) with \( \Delta E_{\text{LH}} \) representing the energy splitting between the LH\(^{(1)}\) and HH\(^{(1)}\) subbands, the holes in the LH\(^{(1)}\) subband are also in the degenerate regime, and thus the effect of the Pauli blocking becomes significant. Consequently \( \tau_{DP} \) decreases with \( N_h \). The second peak appears around the hole density satisfying \( E_F^h - \Delta E_{\text{LH}} = k_B T \).

Then we turn to the case of high impurity density with the impurity density being identical to the hole density. The scenario of the peak is as follows. The SRT due to the DP mechanism increases monotonically with hole density, since the electron–impurity scattering increases with \( N_h \) (= \( N_i \)). Moreover, the SRT due to the BAP mechanism increases with \( N_h \) due to the increase of the hole distribution of the HH\(^{(1)}\) and LH\(^{(1)}\) subbands, similar to the electron–hole Coulomb scattering. As a result, the peak appears around the hole density where the BAP mechanism surpasses the DP mechanism \([20]\). It is also seen that \( \tau_{\text{tot}} \) increases with hole density when \( N_h > 9 \times 10^{11} \, \text{cm}^{-2} \). The underlying physics is as follows. Similar to the previous discussion of the temperature dependence, with the increase of hole density, the decrease of the matrix element \( M_{-1/2,1/2} \) counteracts the increase of the other matrix elements. Thus the dependence of the hole density from the matrix elements is weak. Consequently, when the holes in the HH\(^{(1)}\) and LH\(^{(1)}\) subbands are both in the degenerate regime, the effect of the increase of the Pauli blocking is dominant, and \( \tau_{\text{BAP}} \) increases with \( N_h \). The valley appears around the hole density satisfying \( E_F^h - \Delta E_{\text{LH}} = k_B T \). It is also noted that the increase of \( \tau_{\text{BAP}} \) only appears in the multi-hole-subband calculation. In the single-hole-subband calculation, \( \tau_{\text{BAP}} \) does not increase with \( N_h \) but remains almost a constant for high hole density (the blue dashed curve), since the increase of the Pauli blocking is counteracted by the increase of the matrix elements relevant to the HH\(^{(1)}\) subband.

The hole-density dependence of the spin relaxation at high temperature is also investigated (figure 4(b)). Differing from the behavior at low temperature, it is seen that there is only one

\(^9\) It is also noted that the contribution from the HH\(^{(2)}\) subband is always negligible in this case.
peak in both the impurity-free and high impurity density cases. We further show that the peaks in both cases come from the competition of the DP and BAP mechanisms, which is similar to the peak in the case with high impurity density and low temperature. The absence of the peak from the electron–hole Coulomb scattering is due to the multi-hole-subband effect. As discussed above, when the hole density is high enough so that the holes in the lowest subband are in the degenerate regime, the contribution of the electron–hole Coulomb scattering from the lowest hole subband decreases with increasing hole density due to the increase of Pauli blocking. However, at high temperature the contribution from high hole subbands is also important in this hole-density regime. It is further noted that the holes in the high subbands are still in the nondegenerate regime; thus the contribution from the high hole subbands increases rapidly with \( N_h \) and surpasses the effect from the lowest hole subband. Consequently, \( \tau_{\text{DP}} \) continues to increase with \( N_h \) and the Coulomb peak disappears.

4. Conclusion and discussion

In conclusion, we have performed a comprehensive investigation on electron spin relaxation in p-type GaAs quantum wells from a fully microscopic KSBE approach. All relevant scatterings, such as, electron–impurity, electron–phonon, electron–electron Coulomb, electron–hole Coulomb and electron–hole exchange (the BAP mechanism) scatterings, are explicitly included. We present a phase-diagram-like picture showing the parameter regime where the DP or BAP mechanism is more important. In the case with no impurity and high excitation density, our results are consistent with those in [12]; the BAP mechanism is unimportant at low temperature, which is in stark contrast with the common belief in the literature [1], [7]–[10]. However, by extending the scope of investigation to higher hole density with more hole subbands included, we discover that the BAP mechanism can surpass the DP mechanism in the regime with high temperature and sufficiently high hole density. In cases with low excitation density and/or high impurity density, the regime where the BAP mechanism surpasses the DP mechanism becomes larger. We also show that the temperature regime where the BAP mechanism is more efficient than the DP mechanism is very different in the impurity-free and high impurity density cases. In the impurity-free case, this regime is around the hole Fermi temperature for high hole density, regardless of excitation density. However, in the high impurity density case with identical hole and impurity densities, this regime is roughly from the electron Fermi temperature to the hole Fermi temperature. This is because the dominant scatterings in these two cases are the electron–hole Coulomb scattering and the electron–impurity scattering, respectively. The different dominant scatterings lead to the different temperature dependences of \( \tau_{\text{DP}} \), and hence the different behaviors of the ratio \( \tau_{\text{BAP}} / \tau_{\text{DP}} \). In particular, in the case with high impurity and very low electron excitation densities, the electron (hole) Fermi temperature is much lower than (close to) the lowest (highest) temperature of our investigation. Consequently, the BAP mechanism can dominate the spin relaxation in the whole temperature regime. Moreover, we predict that for the impurity-free case, in the regime where the DP mechanism dominates the spin relaxation, e.g. the cases with high excitation or low hole density, the total SRT presents a peak around the hole Fermi temperature, which is from the nonmonotonic temperature dependence of the electron–hole Coulomb scattering.

The multi-hole-subband effect on spin relaxation is also revealed. It is shown that the multi-hole-subband effect enhances the relative importance of the BAP mechanism significantly for high temperature and/or high hole density. We also predict that at low temperature the spin
relaxation has a very intriguing hole-density dependence, thanks to the contribution from high hole subbands. In the impurity-free case, the total SRT shows a double-peak structure. Both peaks originate from the nonmonotonic hole-density dependence of the electron–hole Coulomb scattering. The only difference is that the first (second) peak comes from the contribution from the HH$^{(1)}$ (LH$^{(1)}$) subband, and hence appears around the hole density satisfying $E_B^H = k_B T$ ($E_B^L \Delta E_{LH^{(1)}} = k_B T$). In the high impurity density case with identical impurity and hole densities, there is first a peak and then a valley. The peak is formed as the DP and BAP mechanisms compete with each other: the SRT due to the DP (BAP) mechanism increases (decreases) with $T$ as the DP (BAP) mechanism dominates at low (high) temperature. Moreover, since the decrease of the matrix element $M_{-1/2,1/2}^L$ counteracts the increase of the other matrix elements of BAP scattering, the hole-density dependence from the matrix elements is weak. Consequently, when the holes in the HH$^{(1)}$ and LH$^{(1)}$ subbands are both in the degenerate regime, the effect of the increase of Pauli blocking is dominant, and $\tau_{\text{BAP}}$ increases with $N_h$. Therefore the valley is formed. However, at high temperature, we show that the peak from the electron–hole Coulomb scattering disappears and only the peak from the competition of the BAP and DP mechanisms remains.

Finally, we discuss the relevance to experiments. Since electrons are minority carriers in p-type semiconductors, they have finite lifetime limited by the electron–hole recombination. From experiments, the electron lifetime is found to be on the order of several hundreds of picoseconds [1, 44], which may be shorter than the SRT in some parameter regimes such as the high impurity density case. However, it has been demonstrated that SRT much longer than the lifetime can be measured via the Hanle or other time-resolved measurements [1, 45]. Hence the calculated long SRTs can be observed in reality. In short, our calculation based on realistic parameters provides useful information in a wide range of experimental conditions, which would benefit the understanding on spin relaxation.

Acknowledgments

This work was supported by the National Natural Science Foundation of China under Grant No. 10725417, the National Basic Research Program of China under Grant No. 2006CB922005 and the Knowledge Innovation Project of Chinese Academy of Sciences.

Appendix. Comparison with experiment

We compare the calculation via the KSBE approach with the experimental results in [44]. In figure A.1, we plot the temperature dependence of the SRTs from our computation and from the experiment in a p-type GaAs quantum well. Here $a = 3 \text{ nm}$, $N_h = 3 \times 10^{11} \text{ cm}^{-2}$ and $N_{ex} = 2.6 \times 10^9 \text{ cm}^{-2}$, as indicated in the experiment [44]. $N_i = 0.3 N_h$ is obtained by fitting the mobility $\mu \simeq 4000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ given in [44]. We take the Dresselhaus spin–orbit coupling parameter as $\gamma_D = 18.3 \text{ eV \AA}^3$. As the range of $\gamma_D$ in bulk GaAs calculated and measured via various methods is from 6.4 to 25.5 eV \AA$^3$ [36], our value of $\gamma_D$ is reasonable. It is seen that our calculation is in good agreement with the experimental data. The deviation at $T = 5 \text{ K}$ is probably because the electron temperature $T_e$ is higher than the lattice temperature $T$ in the experiment due to photo-excitation. This effect becomes significant at low temperature [1, 9]. It is also noted that the SRT due to the BAP mechanism is over one order of magnitude larger than that from the DP one, i.e. the spin relaxation is totally governed by the DP mechanism in
Figure A.1. SRTs $\tau$ from the experimental data in [44] and from the DP and BAP mechanisms calculated via the KSBE approach in a p-type GaAs quantum well.

this case. This is consistent with our conclusion that the BAP mechanism is unimportant at low impurity and hole densities.

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New Journal of Physics **11** (2009) 113039 (http://www.njp.org/)