Nonlinear Rashba model and spin relaxation in quantum wells

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We find that the Rashba spin splitting is intrinsically a nonlinear function of the momentum, and the linear Rashba model may overestimate it significantly, especially in narrow-gap semiconductors. A nonlinear Rashba model is proposed, which is in good agreement with the numerical results from the eight-band $\mathbf{k}\cdot\mathbf{p}$ theory. Using this model, we find pronounced suppression of the D'yakonov-Perel' spin relaxation rate at large electron densities, and a nonmonotonic dependence of the resonance peak position of the electron spin lifetime on the electron density in [111]-oriented quantum wells, both in qualitative disagreement with the predictions of the linear Rashba model.

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Recently, there has been growing interest in the field of spintronics,[1–3] which explores the electron spin, in addition to the electron charge, to realize new functionalities in future electronic devices.[4–6] A promising approach implementing such spintronic devices is to utilize the Rashba spin-orbit interaction caused by structure inversion asymmetry in quantum wells (QW's),[7] which can be controlled by gate voltages[8,9] as well as band-structure engineering.[10,11] Approximate analytical expressions based on second-or third-order perturbation theories[10–12] suggest that the Rashba spin splitting (RSS) is a linear function of the in-plane wave vector $k_\parallel$. This linear Rashba model has been widely used to investigate the various spin-related properties of low-dimensional semiconductor structures, e.g., electron spin relaxation[13–17] and the newly discovered spin Hall effect.[18–24] However, recent numerical calculations[12,25,26] show that the RSS in certain semiconductor QW's deviates from the linear behavior at large $k_\parallel$, although the underlying physics remains unclear. Since the linear Rashba model is still widely used by mainstream researchers, it is important to explore the underlying physics beneath such deviation and, if necessary, check the validity of the linear Rashba model.

In this Brief Report, we find from analytical derivation from the eight-band $\mathbf{k}\cdot\mathbf{p}$ theory that the RSS is intrinsically a nonlinear function of the wave vector, which is caused by the weakening of the interband coupling with increasing kinetic energy of the electron in the conduction band. We show from numerical comparisons that the deviation of the linear Rashba model could be surprisingly large at large wave vectors, especially for narrow-gap semiconductors. These facts substantiate the necessity for a nonlinear Rashba model. We propose such a model, which is in good agreement with the numerical results from the eight-band $\mathbf{k}\cdot\mathbf{p}$ theory for various QW's. This nonlinear Rashba model would lead to a series of significant modifications to the various spin-related properties of the electron, most of which have been investigated based on the linear Rashba model. For example, we find pronounced suppression of the D'yakonov-Perel' (DP) spin relaxation rate (SRR) at large electron density, in qualitative disagreement with the prediction of the linear Rashba model.[15,16] The resonant enhancement of the electron spin lifetime in [111]-oriented quantum wells[17] also exhibits qualitatively different behavior from the linear Rashba model. The values of the SRR obtained by the two models differ by up to several orders of magnitude. Further surprising consequences are expected when this nonlinear Rashba model is applied to other fields.

For [001]-oriented heterostructures, the eight-band Hamiltonian[27] $H=H_k+V$, where $V=eFz$ is the external electric-field induced potential and H_k is the eight-band envelope-function Hamiltonian. Neglecting the off-diagonal elements in the valence bands and eliminating the valence-band components of the envelope function, the effective conduction-band Hamiltonian is obtained as

$$H_{\mathrm{eff}}(k_\parallel)=E_c(z)+V(z)+\mathbf{k}\frac{\hbar^2}{2m^*}\mathbf{k}+\alpha_0(z)(k_\parallel\times e_z)\cdot\sigma, \quad (1)$$

where $\alpha_0=\hbar^2/(6m_0)\partial\gamma(z)/\partial z$, $\gamma(z)=E_P[1/U_{\mathrm{lh}}(z)-1/U_{\mathrm{SO}}(z)]$. $E_P=2m_0P_0^2/\hbar^2$, and m^* is the effective mass given by $m^*=m_0[\gamma_c+2E_P/(3U_{\mathrm{lh}})+E_P/(3U_{\mathrm{SO}})]^{-1}$, $U_{\mathrm{lh}}=E-H_{\mathrm{lh}}$, $U_{\mathrm{SO}}=E-H_{\mathrm{SO}}$, and H_{lh} and H_{SO} are the diagonal elements of the light-hole and spin-orbit split-off bands in the eight-band Hamiltonian. From Eq. (1), we find that the dominant contribution to the RSS consists of the interface term $\Delta E_n^{(1)}$ in the valence band and the external electric-field term $\Delta E_n^{(2)}$,

$$\Delta E_n^{(1)}(k_\parallel)=\frac{\hbar^2}{3m_0}k_\parallel\sum_j|F_n(z_j)|^2[\gamma(z_j^+)-\gamma(z_j^-)], \quad (2)$$

$$\Delta E_n^{(2)}(k_\parallel)=\frac{\hbar^2}{3m_0}E_PeFk_\parallel\int dz|F_n(z)|^2(U_{\mathrm{lh}}^{-2}-U_{\mathrm{so}}^{-2}). \quad (3)$$

Here $F_n(z)$ is the envelope function of the nth subband along the z axis, and $\{z_j\}$ denotes the z coordinates of the interfaces. According to Ehrenfest's theorem, the external electric-field contribution $\Delta E_n^{(2)}$ is approximately canceled by the interface electric-field contribution in the conduction band.[28] As a result, the dominant contribution to RSS comes from the interface term only.[11] From Eq. (2), we see that RSS is approximately inversely proportional to the effective band gap $E_g^{\mathrm{eff}}=E-E_v$, where E_v is the valence-band edge and E is the electron energy. Since the electron energy E increases approximately quadratically as $k_\parallel$ increases, the RSS would always begin to decrease after $k_\parallel$ has exceeded a critical value. This reveals that the previously found deviation of the RSS

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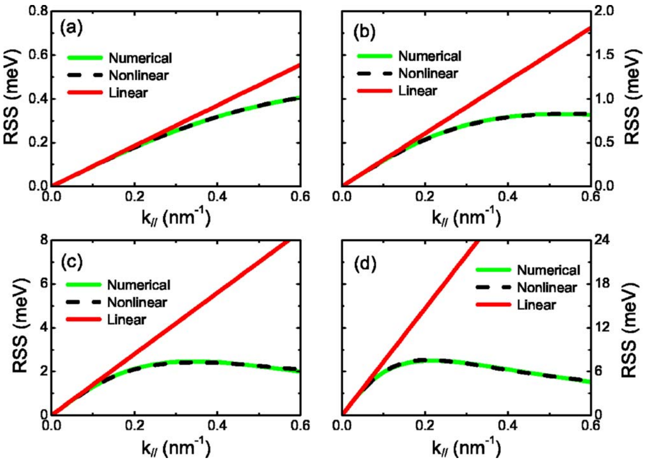

FIG. 1. (Color online) Comparison of the linear (red or dark gray lines) and nonlinear (black lines) models with the numerical results (green or light gray lines) obtained from the eight-band $\mathbf{k}\cdot\mathbf{p}$ theory for the lowest conduction subband of 15-nm-wide (a) $GaAs/Ga_{0.67}Al_{0.33}As$, (b) $Ga_{0.47}In_{0.53}As/Al_{0.48}In_{0.52}As$, (c) $InAs/In_{0.75}Al_{0.25}As$, and (d) $Hg_{0.79}Cd_{0.21}Te/CdTe$ QW's with an electric field 60 kV/cm.

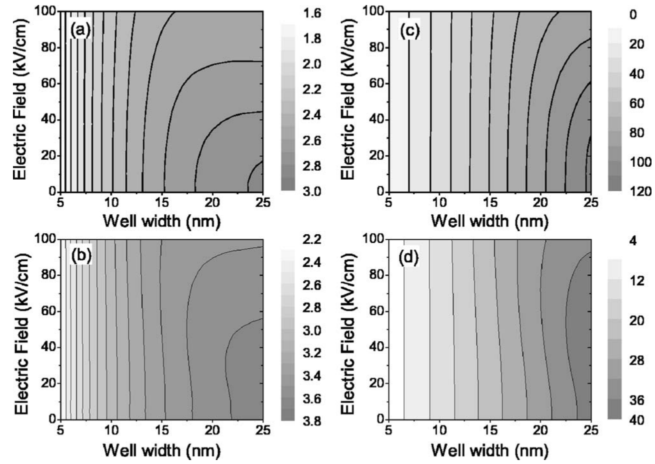

FIG. 2. Rashba coefficient α/F (upper panels) and β (down panels) of the lowest conduction subband as a function of the well width and external electric field for $Ga_{0.47}In_{0.53}As/Al_{0.48}In_{0.52}As$ [(a) and (b)] and $Hg_{0.79}Cd_{0.21}Te/CdTe$ [(c) and (d)] QW's. The units of α/F and β are meV nm/(100 kV/cm) and nm^2, respectively.

from linear behavior in certain QW's[12,25,26] is actually a universal behavior, suggesting that the widely used linear Rashba model needs to be checked and, if necessary, replaced by a nonlinear one.

Enlightened by the above discussions, we propose the following two-coefficient nonlinear Rashba model to describe the RSS of a given subband n,

$$\Delta E_n(k_\parallel) = \frac{2\alpha_n k_\parallel}{1+\beta_n k_\parallel^2}, \tag{4}$$

where α_n is the linear Rashba coefficient of the nth subband for the widely used linear Rashba model $\Delta E_n(k_\parallel)=2\alpha_n k_\parallel$, while $\beta_n k_\parallel^2$ describes the contribution from the kinetic energy of electron in the nth subband. The latter leads to the decrease of RSS when $k_\parallel$ exceeds a critical value $k_0=1/\sqrt{\beta_n}$, which is determined from $\{d[\Delta E_n(k_\parallel)]/dk_\parallel\}_{k_\parallel=k_0}=0$.

In Fig. 1, we compare the linear and nonlinear Rashba models with the numerical results obtained from the eight-band $\mathbf{k}\cdot\mathbf{p}$ theory for different QW's. The band gap of the well material ranges from 1.519 eV (for GaAs) to 0.1 eV (for $Hg_{0.79}Cd_{0.21}Te$). We see that the deviation of the linear model from the numerical results could be surprisingly large, especially for narrow-gap QW's, while the nonlinear model is in good agreement with the numerical results. Thus we substantiate the necessity to use the nonlinear Rashba model instead of the linear one.

To characterize the nonlinear Rashba model, we consider the dependence of the Rashba coefficients α_n and β_n on the various band parameters. To the lowest order, the probability asymmetry at the two interfaces of the QW is proportional to the external electric field F. Then Eq. (2) suggests $\Delta E_n(\mathbf{k}_\parallel) \sim k_\parallel F/[E_g+E_{n0}+\hbar^2k_\parallel^2/(2m_n^*)]$, where E_{n0} is the quantum confining energy and m_n^* is the effective mass of the nth subband. This shows that

$$\alpha_n \sim \frac{F}{E_g+E_{n0}}, \tag{5}$$

$$\beta_n \sim \frac{1}{m_n^*(E_g+E_{n0})}. \tag{6}$$

α_n and β_n both increase with decreasing band gap and subband index n, or increasing well width, i.e., the quantum confining energy E_{n0}. The significant difference is that α_n increases with increasing external electric field F, while β_n is approximately independent of F. Notice, however, that the additional dependence of α_n and β_n on the external electric field may come from the quantum confining energy, especially at large electric fields.

In Fig. 2, we plot the Rashba coefficient α/F and β of the lowest conduction subband (obtained by fitting the results from the eight-band $\mathbf{k}\cdot\mathbf{p}$ theory) as functions of the well width and external electric field for different semiconductor QW's. Some common features can be observed. First, α/F and β are weakly dependent on the external electric field. This shows that α is approximately proportional to the external electric field while β is approximately independent of F, in agreement with Eqs. (5) and (6). Secondly, α/F and β increase with the increase of the well width and begin to saturate at large well width. The saturation value decreases with the increase of the electric field, and this trend becomes increasingly pronounced when the band gap of the well decreases. The increase and saturation behavior comes from the competition between the band gap E_g and the quantum confining energy E_{n0} especially at small well width. The decrease of the saturation values of α/F and β at large well width comes from the enhancement of the quantum confining energy E_{n0} due to the triangular potential induced by the external electric field. It also reflects the fact that the relationship $\alpha \propto F$ begins to break down for wide QW's. Thirdly, the critical well width at which α/F begins to saturate de-

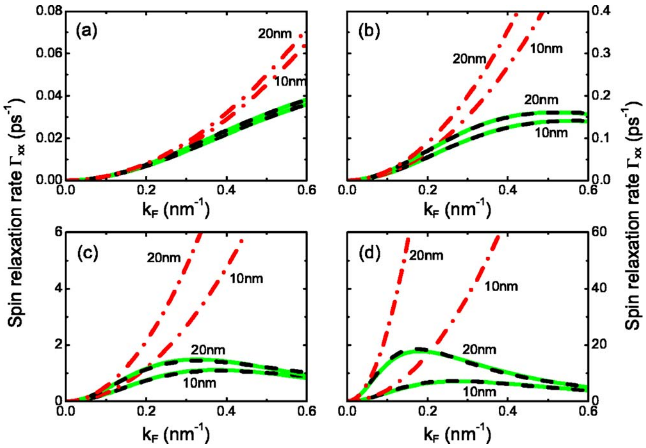

FIG. 3. (Color online) Low-temperature DP SRR in the lowest conduction subband of 20-nm- and 10-nm-wide (a) GaAs/$Ga_{0.67}Al_{0.33}As$, (b) $Ga_{0.47}In_{0.53}As/Al_{0.48}In_{0.52}As$, (c) InAs/$In_{0.75}Al_{0.25}As$, and (d) $Hg_{0.79}Cd_{0.21}Te$/CdTe QW's with an electric field 60 kV/cm and momentum relaxation time 0.1 ps. The results are obtained from the eight-band model (green or light gray lines), and the nonlinear (black lines) and linear (red or dark gray lines) Rashba models, respectively.

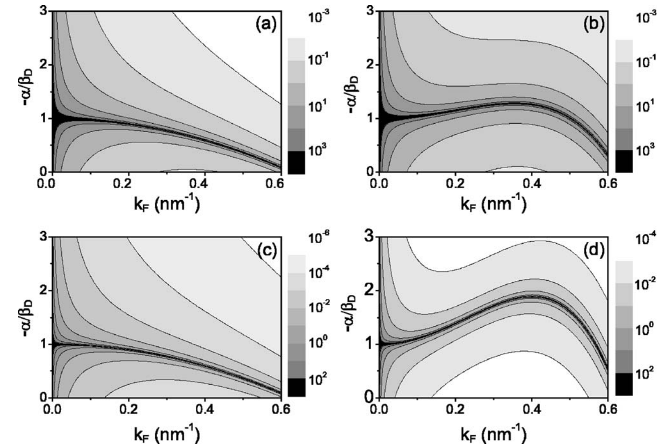

FIG. 4. Spin lifetime (in units of ps) for 10-nm-wide $InAs/In_{0.75}Al_{0.25}As$ [(a) and (b)] and $Hg_{0.79}Cd_{0.21}Te$/CdTe [(c) and (d)] QW's with a typical momentum relaxation time 0.1 ps. The linear (nonlinear) Rashba model is used for (a) and (c) [(b) and (d)].

creases with the increase of the electric field. This can be understood from the competition between the square potential [produced by the conduction-band profile $E_c(z)$] and the triangular potential (produced by the external electric field). With the increase of the well width, the square potential becomes weaker and the triangular potential begins to dominate. This transition occurs at a smaller well width when the external electric field gets stronger, leading to the saturation of the quantum confining energy E_{n0} and, consequently, the Rashba coefficients α/F and β at a smaller well width. The similarities between α/F and β are in agreement with our analytical discussions in Eqs. (5) and (6). However, we should notice that α is approximately linearly dependent on the external electric field F, while β is approximately independent of F.

In the above, we see that the nonlinear Rashba model differs significantly from the linear model. As a result, we expect that this nonlinear Rashba model would lead to a series of modifications to the various spin-related properties of the electron, which have been investigated based on the linear Rashba model.[13–24] As an example, we consider the electron spin relaxation caused by Rashba spin-orbit coupling in two-dimensional electron gas. The electron spin relaxation process has received intensive interest recently because it plays an essential role in the practical application of spintronic devices and quantum information processing.[29–32] For electrons in n-doped semiconductors at large electron density, the DP mechanism is the dominant process and it has been investigated by several groups[15–17] using the linear Rashba model in the framework of the density-matrix formalism. We follow this procedure and calculate the DP SRR [$\Gamma_{xx}=\Gamma_{yy}=\Gamma_{zz}/2$, $\Gamma_{ij}=0(i\neq j)$] using the eight-band $\mathbf{k}\cdot\mathbf{p}$ theory, and the nonlinear and linear Rashba models, respectively. The results for different QW's are shown in Fig. 3. The SRR's from the nonlinear Rashba model show pronounced suppression at large Fermi wave vector k_F (i.e., electron density), in good agreement with the numerical results from the eight-band $\mathbf{k}\cdot\mathbf{p}$ theory, while those from the linear Rashba model increase monotonically with k_F, which qualitatively disagrees with the nonlinear model. The difference between the linear and nonlinear Rashba models increases significantly with the increase of k_F. Taking the 20-nm-wide QW's for example, at $k_F=0.4$ nm^{-1} (corresponding electron density $n_e\approx 2.5\times 10^{12}$ cm^{-2}, which is of interest to, e.g., transport measurements), the relative difference between the two models reaches 40%, 140%, 500%, and 3800% for Figs. 3(a)–3(d), respectively.

In the above, we consider only the Rasbha spin-orbit coupling in order to demonstrate the significant consequences that are introduced by our nonlinear Rasbha model. To perform realistic calculations, however, both the nonlinear Rashba model and the Dresselhaus spin-orbit coupling should be included. Recently it was predicted based on the linear Rashba model that the interplay between the Rashba and Dresselhaus spin-orbit interactions would greatly enhance the electron spin lifetime in [111]-oriented quantum wells when the linear Rashba coefficient α and the linear Dresselhaus coefficient β_D are opposite (i.e., when the ratio $-\alpha/\beta_D=1$).[17] As a second example, we reconsider this problem using the nonlinear Rashba model. The electron spin lifetime τ_{zz} (along the growth direction of the QW) obtained from the two models is compared in Fig. 4 as a function of the ratio $(-\alpha/\beta_D)$ and Fermi wave vector k_F. The black regions correspond to the resonant enhancement regions of the spin lifetime. The most striking feature is that the ratio $(-\alpha/\beta_D)$ at the resonance peak (later referred to as the peak position) shows a nonmotonic dependence on the Fermi wave vector [cf. Figs. 4(b) and 4(d)], which differs qualitatively from the monotonically decreasing behavior of the linear Rashba model [cf. Figs. 4(a) and 4(c)]. Here the monotonic decrease of the peak position with increasing k_F in the linear Rashba model comes from the Dresselhaus k^3 term, while the nonlinearity of the Rashba effect competes against the Dresselhaus k^3 term, leading to nonmonotonic dependence of the peak position on the Fermi wave vector. The values of the spin lifetime obtained from the nonlinear Rashba model also differ from the prediction of the linear Rashba model by up to several orders of magnitude [cf. Figs. 4(c) and 4(d)].

In summary, we have revealed that the RSS in semiconductor QW's is intrinsically a nonlinear function of the wave vector. It may be overestimated significantly by the linear Rashba model, especially in narrow-gap QW's. We propose a two-coefficient nonlinear Rashba model, which is in good agreement with the numerical results obtained from the eight-band $\mathbf{k}\cdot\mathbf{p}$ theory. Using this nonlinear model, we found pronounced suppression of the DP SRR at large electron density, and a nonmonotonic dependence of the ratio $(-\alpha/\beta_D)$ at the resonance peak of the electron spin lifetime on the Fermi wave vector in [111]-oriented QW's, both in qualitative disagreement with the predictions of the linear Rashba model. The values of the spin lifetime obtained from the two models may differ by up to several orders of magnitude. Further surprising results are expected when the nonlinear Rashba model is applied to other fields.

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