Anomalous Rashba spin splitting in two-dimensional hole systems

R. Winkler
Institut für Technische Physik III, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

H. Noh, E. Tutuc, and M. Shayegan
Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544
(Received 4 September 2001; published 20 March 2002)

It has long been assumed that the inversion asymmetry-induced Rashba spin splitting in two-dimensional (2D) systems at zero magnetic field is proportional to the electric field that characterizes the inversion asymmetry of the confining potential. Here we demonstrate, both theoretically and experimentally, that 2D heavy hole systems in accumulation-layer-like single heterostructures show the opposite behavior; i.e., a decreasing, but nonzero electric field results in an increasing Rashba coefficient.

DOI: 10.1103/PhysRevB.65.1553XX PACS number(s): 73.21.−b, 71.70.Ej

Spin degeneracy of electron and hole states in a solid stems from the inversion symmetry in space and time. If the spatial inversion symmetry is broken, then there is a splitting of the single-particle states even at magnetic field $B=0$ (Ref. 1). In quasi-two-dimensional (quasi-2D) semiconductor structures, the bulk inversion asymmetry (BIA) of the underlying crystal structure (e.g., a zinc blende structure) and the structure inversion asymmetry (SIA) of the confining potential contribute to the $B=0$ spin splitting.[2] While BIA is fixed, the so-called Rashba spin splitting[3] due to SIA can be tuned by means of external gates that change the electric field **E** in the sample.[4,5] The $B=0$ spin splitting is of significant current interest both because of its fundamental importance and its possible device applications.[6]

For many years it has been assumed that the Rashba spin splitting in 2D systems is proportional to the electric field that characterizes the inversion asymmetry of the confining potential.[2,4–9] In single heterostructures, where SIA is the dominant source of spin splitting, the electric field is determined by the density-dependent self-consistent potential.[10] One would thus expect that the spin splitting decreases with density, although for 2D electron systems this effect may partly be compensated by many-particle effects that tend to increase the Rashba spin splitting for low densities.[11] Here we demonstrate, both theoretically and experimentally, that 2D heavy hole systems in accumulation-layer-like single heterostructures show the opposite behavior; namely, a decreasing, but nonzero electric field results in an increasing Rashba coefficient. Contrary to electrons, however, exchange-correlation effects in the low-density regime decrease the spin splitting. We show that this surprising result is a consequence of heavy-hole–light-hole (HH-LH) coupling in 2D hole systems. Our findings are particularly remarkable because in HH systems we have essentially a cubic dependence of spin splitting on the in-plane wave vector (as opposed to a linear dependence in electron and LH systems) which implies that, in general, spin splitting decreases even faster when the density is reduced.[7] We obtain good qualitative agreement between calculated and measured spin splittings in 2D hole systems in GaAs heterostructures where the density and spin splitting are varied by means of an external gate. Our results are applicable to many systems, as most III-V semiconductors have essentially the same band structure that is underlying our investigation.

To lowest order of the wave vector **k** and electric field **E**, the SIA spin splitting of electron states in the Γ_6^c conduction band is given by the Rashba term[3]

$$H_{6c}^{\mathrm{SO}}=\alpha\mathbf{k}\times\mathbf{E}\cdot\boldsymbol{\sigma}. \tag{1}$$

Here $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ denotes the Pauli spin matrices and α is a material-specific prefactor.[2] We assume $\mathbf{E}=(0,0,E_z)$. Treating the off-diagonal $\mathbf{k}\cdot\mathbf{p}$ coupling between electron and hole states by third-order Löwdin perturbation theory,[12] we obtain for the Rashba coefficient α_λ of the lowest electron subband $\lambda=1$

$$\alpha_1=eP^2a\left(\frac{1}{\Delta_{11}^{cl}}\frac{1}{\Delta_{12}^{cl}}-\frac{1}{\Delta_{11}^{cs}}\frac{1}{\Delta_{12}^{cs}}\right), \tag{2}$$

where P is Kane's momentum matrix element[13] and $\Delta_{\lambda\lambda'}^{\nu\nu'}\equiv\mathcal{E}_\lambda^\nu-\mathcal{E}_{\lambda'}^{\nu'}$ with $\mathcal{E}_\lambda^c$, $\mathcal{E}_\lambda^h$, $\mathcal{E}_\lambda^l$, and $\mathcal{E}_\lambda^s$ the energy of the λth electron, HH, LH, and split-off subband, respectively.[14] The numerical prefactor a depends on the geometry of the confining quantum well (QW). In an infinitely deep rectangular QW we have $a=256/(81\pi^2)$. For other geometries it has the same order of magnitude. According to Eq. (1) we obtain a spin splitting $\pm\alpha E_z k_\parallel$ of the subband dispersion $\mathcal{E}(\mathbf{k}_\parallel)$ that is proportional to the electric field E_z and is linear in the in-plane wave vector $\mathbf{k}_\parallel=(k_x,k_y,0)$. A detailed analysis reveals that spin splitting of electron states depends on the electric field E_v in the valence band that differs from the electric field E_c in the conduction band by the contributions of the interfaces.[8,9] However, the important point here is that in a single heterostructure both E_v and E_c are determined by the self-consistent Hartree potential.

For hole systems in the Γ_8^v valence band (point group T_d), the dominant contribution to Rashba spin splitting is given by the term[7]

$$H_{8v}^{\mathrm{SO}}=\beta\mathbf{k}\times\mathbf{E}\cdot\mathbf{J}, \tag{3}$$

where β is a system-dependent prefactor and $\mathbf{J}=(J_x,J_y,J_z)$ are the angular momentum matrices for j

$=3/2$. We neglect here the small corrections in H_{8v}^{SO} due to the $\mathbf{k}\cdot\mathbf{p}$ coupling to remote bands such as the higher Γ_8^c and Γ_7^c conduction bands. Quantum confinement splits the fourfold-degenerate Γ_8 valence band into HH and LH states. To lowest order in k the effective Rashba Hamiltonian for the LH states is the same as in Eq. (1) for electron states. For HH states, however, spin splitting is mediated by a coupling to the LH states so that, to lowest order, spin splitting of HH states is of third order in $\mathbf{k}$ (Ref. 7). Neglecting anisotropic corrections in the Hamiltonian we have

$$H_h^{\mathrm{SO}}=\beta^h E_z(\sigma_+ k_-^3+\sigma_- k_+^3), \tag{4}$$

with $\sigma_\pm=1/2(\sigma_x\pm i\sigma_y)$ and $k_\pm=k_x\pm ik_y$. Treating the off-diagonal HH-LH coupling by third-order Löwdin perturbation theory[12] we obtain for the Rashba coefficient β_λ^h of the lowest HH subband $\lambda=1$

$$\beta_1^h=ia\gamma_3(\gamma_2+\gamma_3)\left[\frac{1}{\Delta_{11}^{hl}}\left(\frac{1}{\Delta_{12}^{hl}}-\frac{1}{\Delta_{12}^{hh}}\right)+\frac{1}{\Delta_{12}^{hl}\Delta_{12}^{hh}}\right], \tag{5}$$

where γ_2 and γ_3 are the Luttinger parameters.[15] In an infinitely deep rectangular QW we have $a=64/(9\pi^2)$. We see from Eq. (5) that the Rashba spin splitting of HH states depends not only on the electric field E_z but also on the separation between the HH and LH subbands. A decreasing separation gives rise to an increasing Rashba coefficient β_1^h. The factor $\gamma_3(\gamma_2+\gamma_3)$ in Eq. (5) refers to a quantum structure grown in the crystallographic direction [001]. The expressions for other growth directions are similar, but the other terms in Eq. (5) remain unchanged. We remark that for typical hole densities only the lowest HH subband is occupied.

The electric field E_z that enters into the Rashba Hamiltonian depends on the charges in the system. We will show now that accumulation-layer-like single heterostructures behave rather differently with respect to changes of the 2D charge density as compared to other quasi-2D semiconductor structures.

In a rectangular QW, a small density N and a small asymmetry imply that the properties of the system are controlled by the effective potential steps at the interfaces; i.e., changes in N or E_z have a minor effect in this regime. In an inversion-layer-like heterostructure, we always have a band bending of the order of the fundamental gap so that, for small densities, the Hartree potential and E_z are determined by the space charges due to the given concentration of ionized majority impurities in the system. For accumulation-layer-like systems, on the other hand, it was shown by Stern,[16] that the space charge layer is controlled by the much smaller concentration of minority impurities in the system. Thus, even for a small 2D density, the dominant contribution to the Hartree potential stems from the charges in the 2D system itself. Therefore, over a wide range of densities N, the electric field E_z is proportional to N. In single heterostructures, the subband separations are approximately proportional to E_z. Using the triangular well approximation[10] we have, for the subband energies $\mathcal{E}_\lambda^\nu$ measured from the corresponding bulk band edge, $\mathcal{E}_\lambda^\nu\propto E_z^{2/3}$ which implies $\mathcal{E}_\lambda^\nu\propto N^{2/3}$ and $\beta_\lambda^h\propto N^{-4/3}$. Therefore, we can expect from Eqs. (4) and (5) that accumulation-layer-like 2D HH systems show a Rashba spin splitting that increases when N and E_z are reduced. On the other hand, the coefficient (2) is essentially independent of N and E_z because the energy gaps $\Delta_{\lambda\lambda'}^{\nu\nu'}$ are always of the order of the fundamental gap.[14]

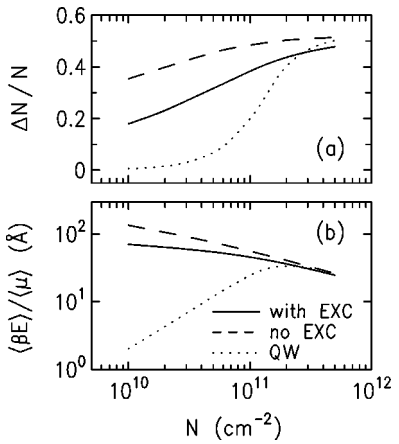

FIG. 1. (a) Spin splitting $\Delta N/N$ and (b) effective spin splitting coefficient $\langle\beta_1^h E_z\rangle/\langle\mu_h\rangle$ as a function of N for a 2D HH system in the accumulation layer of a GaAs-$Al_{0.5}Ga_{0.5}$As single heterostructure on a (001) GaAs substrate, calculated including exchange-correlation (EXC, solid lines) and neglecting exchange-correlation (dashed lines). For the dotted lines see text.

In order to validate these qualitative arguments we present next the results of realistic, fully self-consistent subband calculations.[17] We use an 8×8 multiband Hamiltonian[13] that includes the lowest conduction band Γ_6^c, the topmost valence band Γ_8^v, and the split-off valence band Γ_7^v. The simpler 4×4 Luttinger Hamiltonian,[15] taking into account only the band Γ_8^v, gives essentially the same results. We have checked that higher conduction bands have a minor influence. Many-particle effects are taken into account based on a density-functional approach.[18] From these calculations we obtain the difference $\Delta N=N_+-N_-$ between the spin subband densities $N_\pm$ as a function of the total density $N=N_+ +N_-$.

In Fig. 1(a) we show $\Delta N/N$ calculated as a function of N for a 2D HH system in the accumulation layer of a GaAs-$Al_{0.5}Ga_{0.5}$As single heterostructure on a (001) GaAs substrate.[19] From $N=5\times10^{11}$ cm^{-2} to 1×10^{10} cm^{-2} the parameter r_s, the Coulomb energy to Fermi energy ratio, increases from 4.3 to 17. Therefore, one can expect that many-particle effects are quite important in this regime of densities N. Indeed, we find that taking into account exchange correlation (solid lines) reduces $\Delta N/N$ as opposed to a calculation without exchange correlation (dashed lines). This behavior, which is opposite to 2D electron systems,[11] can be traced back to the fact that exchange correlation increases the subband spacings[18] so that the Rashba coefficient β_1^h is reduced, in agreement with Eq. (5).

It is convenient to characterize our numerical results in terms of an effective Rashba coefficient $\langle\beta_1^h E_z\rangle$ (Ref. 20). Assuming that the spin-split HH subband dispersion is ap-

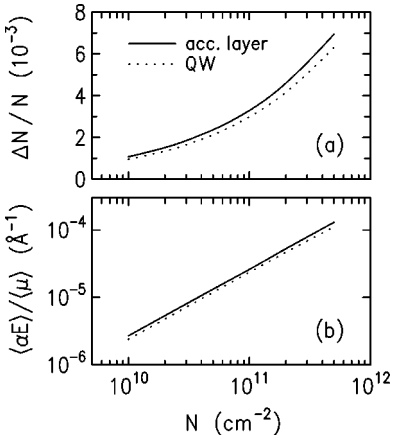

FIG. 2. (a) Spin splitting $\Delta N/N$ and (b) effective spin splitting coefficient $\langle \alpha_1 E_z\rangle/\langle \mu_c\rangle$ as a function of N for a 2D electron system in the accumulation layer of a $Ga_{0.47}In_{0.53}As$-$Al_{0.47}In_{0.53}As$ single heterostructure (solid lines). For the dotted lines see text.

proximately of the form $\mathcal{E}^h_\pm(k_\parallel)=\langle \mu_h\rangle k_\parallel^2 \pm \langle \beta_1^h E_z\rangle k_\parallel^3$, where μ_h (times $2/\hbar^2$) is the reciprocal effective mass, we have

$$\langle \beta_1^h E_z\rangle = \sqrt{\frac{2}{\pi}}\langle \mu_h\rangle \frac{N(\tilde{N}_+ - \tilde{N}_-)+\Delta N(\tilde{N}_+ + \tilde{N}_-)}{6N^2+2\Delta N^2}, \quad (6)$$

with $\tilde{N}_\pm = \sqrt{N \pm \Delta N}$. Figure 1(b) shows that $\langle \beta_1^h E_z\rangle/\langle \mu_h\rangle$ increases when N is reduced.

For comparison, we have calculated $\Delta N/N$ for a 2D electron system in the accumulation layer of a $Ga_{0.47}In_{0.53}As$-$Al_{0.47}In_{0.53}As$ single heterostructure [Fig. 2(a)]. Here spin splitting is given by Eq. (1). Therefore, the spin-split subband dispersion is approximately of the form $\mathcal{E}^c_\pm(k_\parallel)=\langle \mu_c\rangle k_\parallel^2 \pm \langle \alpha_1 E_z\rangle k_\parallel$, and we obtain similarly to Eq. (6) (Ref. 21)

$$\langle \alpha_1 E_z\rangle = \sqrt{2\pi}\langle \mu_c\rangle(\tilde{N}_+ - \tilde{N}_-). \quad (7)$$

In Fig. 2(b) it can be seen that, in contrast to Fig. 1(b), the spin splitting coefficient $\langle \alpha_1 E_z\rangle/\langle \mu_c\rangle$ decreases rapidly with decreasing N. We remark that unlike the HH system in Fig. 1, exchange correlation has only a weak influence on the electron system in Fig. 2 (Ref. 22).

To further analyze our numerical results, we define an effective electric field $\langle E_z\rangle=\langle \partial_z V_H(z)\rangle$, where $V_H(z)$ is the Hartree potential without the effective potential due to the position-dependent band edges. In an accumulation layer the contribution of the space charge layer to $V_H(z)$ is very small.[16] It follows then, by partial integration of the Poisson equation, that $\langle E_z\rangle = e/(2\varepsilon\varepsilon_0)N$, where ε is the dielectric constant and the expectation value refers to the 2D charge density that gives rise to $V_H(z)$. Using these values for $\langle E_z\rangle$ and $\langle \mu_c\rangle = 89$ eV Å^2 we obtain $\langle \alpha_1\rangle \approx 34.3$ e Å^2 independent of N, consistent with Eq. (2). This implies that in Fig. 2(b) the drastic change of $\langle \alpha_1 E_z\rangle/\langle \mu_c\rangle$ merely reflects the change of the electric field $\langle E_z\rangle$. On the other hand, the weak variation of $\langle \beta_1^h E_z\rangle/\langle \mu_h\rangle$ in Fig. 1(b) indicates that the ''bare'' Rashba coefficient $\langle \beta_1^h\rangle$ increases by a factor of 250 when N is lowered from 5×10^{11} to 1×10^{10} cm^{-2} (Ref. 23).

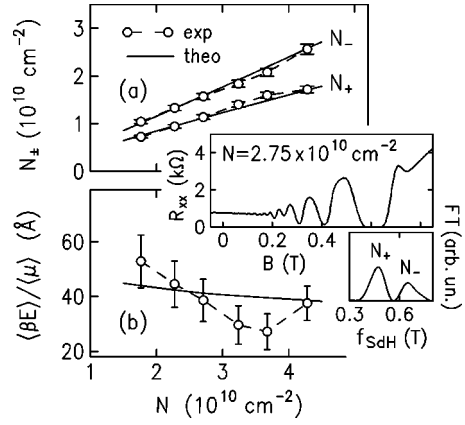

FIG. 3. Measured (circles) and calculated (solid lines) spin subband densities $N_\pm$ (a) and effective spin splitting coefficient $\langle \beta_1^h E_z\rangle/\langle \mu_h\rangle$ (b) as a function of density $N=N_+ + N_-$ for a 2D HH system at a GaAs-$Al_{0.3}Ga_{0.7}As$ single heterostructure on a nominally undoped (311)A GaAs substrate with a weak p-type background doping. The inset shows the measured magnetoresistance R_{xx} as a function of magnetic field B (upper part) and the Fourier transform (FT) of R_{xx} (lower part) for $N=2.75\times10^{10}$ cm^{-2}.

This is in good, qualitative agreement with the analytical model discussed above that predicts an increase of β_1^h by a factor of $50^{4/3}\approx 184$. Note that for low densities the third-order perturbation approach, which underlies Eqs. (2) and (5), breaks down because the subbands are merging together so that higher-order corrections become important. These higher-order terms are fully taken into account in our numerical calculations.[7,17] We remark that the limit of a vanishing electric field implies also that the HH and LH states become degenerate. Therefore, in this limit one must go back from Eqs. (4) and (5) to the more complex Eq. (3). However, for very low densities below 10^{10} cm^{-2} the Hartree potential and spin splitting are ultimately controlled by the fixed concentration of minority impurities.[16,19]

It is interesting to compare the spin splittings in accumulation layers with those in QW's where E_z is tuned externally, e.g., by means of gates.[5] The dotted lines in Figs. 1 and 2 show the calculated results for a 200-Å-wide rectangular QW where the external electric field $E_z^{\rm ext}$ was chosen according to $E_z^{\rm ext}(N)=e/(2\varepsilon\varepsilon_0)N$. In an electron system (Fig. 2) we obtain spin splittings very close to the results for the accumulation layer. In particular, we have $\langle \alpha_1\rangle \approx 30.6$ e Å^2 independent of N. Similarly, for a 2D HH system in a QW (Fig. 1) and $N \lesssim 1\times10^{11}$ cm^{-2} we obtain $\langle \beta_1^h\rangle \approx 7.54 \times 10^6$ e Å^4. [For larger densities higher order corrections in $\mathcal{E}^h_\pm(k_\parallel)$ become important.[7]] Since in QW's the subband spacings are essentially determined by the QW width (i.e., are independent of N), this is consistent with Eq. (5). These calculations also indicate that for 2D HH systems in a QW, spin splitting becomes negligible in the regime of low densities,[7] which is due to the fact that spin splitting of $\mathcal{E}^h_\pm(k_\parallel)$ is proportional to $k_\parallel^3$. However, for 2D HH systems in single heterostructures, spin splitting can be very important in the low-density regime. We note that inversion layers give results similar to QW's, but the specific numbers depend on the details of the doping profile.

In order to reinforce our conclusions, we present next a comparison between measured and calculated spin splittings in a GaAs-$Al_{0.3}Ga_{0.7}As$ single heterostructure grown on a nominally undoped (311)*A* GaAs substrate with a weak *p*-type background doping.[19] A back gate was used to tune the density N from 1.8×10^{10} to 4.2×10^{10} cm^{-2}. To measure the spin subband densities $N_{\pm}$, the Shubnikov–de Haas (SdH) oscillations at low magnetic fields B were examined[4,5] at a temperature $T\simeq50$ mK (see inset of Fig. 3). The frequencies f_{SdH} of these oscillations are a measure of the zero-B spin splitting.[24] In Fig. 3(a) we present the measured and calculated spin subband densities exhibiting remarkably close agreement. Figure 3(b) shows $\langle\beta_1^h E_z\rangle/\langle\mu_h\rangle$ determined by means of Eq. (6). On average, $\langle\beta_1^h E_z\rangle/\langle\mu_h\rangle$ increases as the density is reduced. Taking into account the orders-of-magnitude change that we have for $\langle\beta_1^h E_z\rangle/\langle\mu_h\rangle$ in QW's and for $\langle\alpha_1 E_z\rangle/\langle\mu_c\rangle$ in electron systems, the agreement between experiment and theory is quite satisfactory.[25] We wish to emphasize that it is indeed the anomalous enhancement of the Rashba coefficient in 2D HH systems in accumulation-layer-like single heterostructures that allows us to experimentally resolve the spin splitting in this density regime. Data on QW samples with comparable densities reveal no measurable spin splitting,[26] consistent with the solid and dotted lines in Fig. 1.

Support from the NSF, DOE, and Humboldt Foundation is gratefully acknowledged.

[1] C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963).
[2] U. Rössler, F. Malcher, and G. Lommer, in *High Magnetic Fields in Semiconductor Physics II*, edited by G. Landwehr (Springer, Berlin, 1989), p. 376.
[3] Y.A. Bychkov and E.I. Rashba, J. Phys. C **17**, 6039 (1984).
[4] J. Nitta *et al.*, Phys. Rev. Lett. **78**, 1335 (1997).
[5] S.J. Papadakis *et al.*, Science **283**, 2056 (1999).
[6] *Proceedings of the International Conference on the Physics and Applications of Spin-Related Phenomena in Semiconductors* [Physica E **10**, issues 1–3 (2001)].
[7] R. Winkler, Phys. Rev. B **62**, 4245 (2000).
[8] R. Lassnig, Phys. Rev. B **31**, 8076 (1985).
[9] E.A. de Andrada e Silva, G.C. La Rocca, and F. Bassani, Phys. Rev. B **55**, 16 293 (1997).
[10] F. Stern, Phys. Rev. B **5**, 4891 (1972).
[11] G.-H. Chen and M.E. Raikh, Phys. Rev. B **60**, 4826 (1999).
[12] G. L. Bir and G. E. Pikus, *Symmetry and Strain-Induced Effects in Semiconductors* (Wiley, New York, 1974).
[13] H.-R. Trebin, U. Rössler, and R. Ranvaud, Phys. Rev. B **20**, 686 (1979).
[14] Equation (2) is essentially equivalent to Eq. (3.102a) in E. L. Ivchenko and G. E. Pikus, *Superlattices and Other Heterostructures*, 2nd ed. (Springer, Berlin, 1997). The latter equation describes Rashba spin splitting in a quasibulk material.
[15] J.M. Luttinger, Phys. Rev. **102**, 1030 (1956).
[16] F. Stern, Phys. Rev. Lett. **33**, 960 (1974).
[17] R. Winkler and U. Rössler, Phys. Rev. B **48**, 8918 (1993).
[18] F. Stern and S. Das Sarma, Phys. Rev. B **30**, 840 (1984).
[19] For a concentration of charged minority impurities $N_{\mathrm{min}}\leq5\times10^{13}$ cm^{-3} our results are essentially independent of N_{min}.
[20] We use angular brackets to indicate that the numerical calculation involves an averaging over position-dependent quantities.
[21] Equation (7) differs from the approximate results by G. Engels *et al.* [Phys. Rev. B **55**, R1958 (1997)]. The latter results are correct only up to first order of ΔN.
[22] It was shown in Ref. 11 that the exchange-induced enhancement of the Rashba coefficient α becomes important for $r_s\gtrsim8$. In 2D electron systems we have the largest Rashba spin splitting for semiconductors such as InAs with a small effective mass (i.e., small r_s). For typical densities we have $r_s\lesssim3$ so that usually many-particle corrections can be neglected for α in 2D electron systems. For the system in Fig. 2 we have $r_s=0.5$–3.4.
[23] According to our numerical calculations $\langle\mu_h\rangle$ decreases from 19.1 to 10.7 eV Å^2 for N from 1×10^{10} to 5×10^{11} cm^{-2}.
[24] This association may not be exact; i.e., f_{SdH} multiplied by (e/h) can deviate slightly from the spin subband densities [R. Winkler *et al.*, Phys. Rev. Lett. **84**, 713 (2000)].
[25] We estimate that the experimental error in $N_{\pm}$ is of the order of $\pm4\%$, giving an error in ΔN and $\langle\beta_1^h E_z\rangle/\langle\mu_h\rangle$ of the order of $\pm20\%$. The apparent increase of $\langle\beta_1^h E_z\rangle/\langle\mu_h\rangle$ at $N=4.2\times10^{10}$ cm^{-2} might be a result of experimental uncertainty.
[26] E. Tutuc *et al.*, Phys. Rev. Lett. **86**, 2858 (2001).