Temperature dependence of the electron spin g factor in GaAs

W. Zawadzki*, P. Pfeffer
Institute of Physics, Polish Academy of Sciences
Al. Lotnikow 32/46, 02–668 Warsaw, Poland

R. Bratschitsch**, Z. Chen, S. T. Cundiff
JILA, National Institute of Standards and Technology and University of Colorado,
Boulder, Colorado 80309-0440, USA

B. N. Murdin
Advanced Technology Institute, University of Surrey,
Guildford GU2 7XH, United Kingdom

C. R. Pidgeon
Department of Physics, Heriot-Watt University,
Edinburgh EH14 4AS, United Kingdom

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The temperature dependence of the electron spin g factor in GaAs is investigated experimentally and theoretically. Experimentally, the g factor was measured using time-resolved Faraday rotation due to Larmor precession of electron spins in the temperature range between 4.5 K and 190 K. The experiment shows an almost linear increase of the g value with the temperature. This result is in good agreement with other measurements based on photoluminescence quantum beats and time-resolved Kerr rotation up to room temperature. The experimental data are described theoretically taking into account a diminishing fundamental energy gap in GaAs due to lattice thermal dilatation and nonparabolicity of the conduction band calculated using a five-level kp model. At higher temperatures electrons populate higher Landau levels and the average g factor is obtained from a summation over many levels. A very good description of the experimental data is obtained indicating that the observed increase of the spin g factor with the temperature is predominantly due to band’s nonparabolicity.

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I. INTRODUCTION

The temperature dependence of the spin g value of electrons in GaAs has been a subject of controversy since 1995, when it was shown that the experimental data, exhibiting an increase of the value of g as a function of temperature, are in a qualitative disagreement with the kp theory, if one takes into account an experimental change of the fundamental energy gap [1]. The seeming qualitative disagreement between the experiment and the theory was confirmed by subsequent publications [2, 3]. The temperature dependence of the spin properties of electrons in GaAs is not only of academic interest since for possible spintronic applications the behavior of g near room temperature is clearly of great importance. It was recently shown that one can reach at least a qualitatively correct description of the experimental g values if one includes in the kp theory not the complete temperature change of the fundamental energy gap but the change due to lattice dilatation alone [4]. A similar result was obtained for the g value of electrons in InSb indicating that the better description was not fortuitous.

The experiments [1-3] and their analysis presented in Ref. [4] have two shortcomings. On the experimental side, the g value data was obtained by time-resolved photoluminescence alone, while it would be desirable to verify these data by some other method. On the theoretical side, the analysis in Ref. [4] is somewhat tentative as it does not account for the fact that at higher temperatures electrons populate many Landau levels, so that the measured spin g value represents an average over many transitions. Recognizing the importance of the subject and its controversial character the present work tries to overcome the above shortcomings in both experimental and theoretical aspects. First, we present new data on the temperature dependence of the electron g value in GaAs obtained with the time-resolved Faraday rotation and compare them with the photoluminescence data of

* e-mail address: zawad@ifpan.edu.pl
** Present address: University of Konstanz and Center for Applied Photonics, D-78457 Konstanz, Germany
The paper is organized as follows. We first describe new experiments on the temperature dependence of the electron $g$ value in GaAs. Next, we describe the theoretical procedure used to evaluate the temperature dependence of the $g$ value and compare the theory with all existing experimental data. We discuss our results and conclude the paper by a summary.

II. EXPERIMENT AND THEORY

The spin $g$ factor of electrons in a nominally undoped 30 $\mu$m thick layer of GaAs was determined using an ultrafast degenerate setup for measuring the time-resolved Faraday rotation [5-7]. Spin polarized electrons were optically excited by a circularly polarized pump pulse which was spectrally tuned to the band gap of GaAs at all temperatures. After the excitation the electron spins begin to precess in a magnetic field applied parallel to the sample surface in the Voigt geometry. By measuring the Faraday rotation of a linearly polarized probe beam transmitted through the sample one is able to monitor the electron spin dynamics. The Larmor spin precession results in an oscillating signal that decays exponentially at a rate $1/T_2^*$, where $T_2^*$ is the ensemble spin dephasing time (Fig. 1). The $g$ factor is determined using the equation of Larmor precession: $g^* = h\omega_L/\mu_BB$, where $\omega_L$ is the measured Larmor precession frequency, $\mu_B$ is the Bohr magnetron, and $B$ is the applied magnetic field. The ultrafast femtosecond laser pulses ($\Delta \lambda = 15.5$ nm, $P_{\text{pump}} = 10$ mW, $P_{\text{probe}} = 1$ mW) were generated by a mode-locked Ti:sapphire laser operating at 76 MHz repetition frequency. The samples were held at low temperatures using an optical cryostat and a magnetic field was generated by a split-coil superconducting magnet. Magnetic fields up to 6 T have been applied.

GaAs is a medium-gap material, so that a three-level $k\mathbf{p}$ description, successfully used for narrow gap semiconductors [8, 9], is not adequate for treating its band structure. The reason is that in GaAs the fundamental gap $E_0$ between the $\Gamma_6^v$ and $\Gamma_8^c$ levels is about 1.5 eV, i.e. it is not much smaller than the gap $E_1$ between the $\Gamma_6^v$ level and the upper $\Gamma_7^c$ conduction level (which is about 3 eV). It has been convincingly demonstrated that an adequate way to treat the conduction band of GaAs is to use a five-level model (5LM, which is equivalent to 14 bands including spin) in the $k\mathbf{p}$ description (see Refs. [10, 11] and the references therein). In particular, for the description of electron spin $g$ value in GaAs-based heterostructures the usefulness of the 5LM was demonstrated quite recently [12]. Since the 5LM for electrons in the presence of a magnetic field and its use for magneto-optical properties of GaAs was described in some details before [10, 11], we only mention here the main elements of this approach. Thus the model includes exactly the $\Gamma_7^v$, $\Gamma_8^c$, $\Gamma_6^v$, $\Gamma_7^v$ and $\Gamma_5^v$ levels at the center of the Brillouin zone and the resulting $k\mathbf{p}$ matrix has dimensions $14 \times 14$. There exist three nonvanishing interband matrix elements of momentum: $P_0$, $P_1$ and $Q$, and one interband element of the spin-orbit interaction $\Delta$. If one takes $Q = 0$ and $k_z = 0$ (where $k_z$ is the momentum along the magnetic field direction) the $14 \times 14$ initial matrix factorizes into two $7 \times 7$ matrices for the spin-up and spin-down states. These matrices are soluble with the envelope functions in the form of harmonic oscillator functions and the eigenenergies for different Landau levels (LLs) $n$ reduces to a diagonalization of $7 \times 7$ determinants. However, if the $Q$ element is included (it comes from an inversion asymmetry of the GaAs crystal) the initial $14 \times 14$ matrix does not factorize and it is not soluble in terms of a single column of harmonic oscillator functions. Physically, this means that the resulting energy bands are not spherical. Since the nonsphericity of the conduction band in GaAs is small, one can solve for the eigenenergies looking for the envelope functions in terms of sums of harmonic oscillator functions. This leads to number determinants composed of the fundamental $7 \times 7$ blocks on the diagonal coupled by nondiagonal parts involving the $Q$ elements. The eigenenergies are computed truncating the resulting big determinants. In our computations we used typically 21 $\times$ 21 determinants. All calculations were performed taking the magnetic field $B$ parallel to [001] direction and putting $k_z = 0$.

Now we turn to the temperature dependence of the fundamental gap $E_0$. It was argued a long time ago [13] and confirmed by the behavior of the effective mass [14, 15] that the temperature dependence of the band parameters is governed by a dilatational change of the energy gap $E_0$ and not by its total (i.e. measured) change. The other contribution to the change of the gap is due to phonons.
However, the phonon vibrations occur on a much slower time scale than the time the electron needs to sample the interband interactions determining the effective mass and the $g$ factor, which are at optical frequencies. The dilatational change of the gap is given by [16]

$$\Delta E_0^{dl}(T) = -3D \left( \frac{\partial E}{\partial P} \right)_T \int_0^T \alpha_{th}(T')dT', \quad (1)$$

where $D$ is the bulk modulus, $dE/dP$ is the pressure-induced band-gap shift, and $\alpha_{th}(T)$ is the linear thermal expansion coefficient (see also [17]). The quantities $B$ and $\partial E/\partial P$ are readily measurable, the quantity $\alpha_{th}(T)$ was measured for GaAs by Novikova [18] and Soma et al [19]. Using the values of $\alpha_{th}(T)$ one calculates $\Delta E_0^{dl}(T)$. This was done by Lourenco et al [16], we replot their results in Fig. 2. It should be mentioned that $\alpha_{th}(T)$ goes through a minimum near $T \approx 50$ K, this results in a plateau and a flat maximum of $E_0^{dl}(T)$ seen in Fig. 2. The dilatational change $\Delta E_0^{dl}$ of the fundamental gap between 0 K and 300 K is about 23 meV (see Fig. 2), while the total change $\Delta E_0^{tot}$ is about 93 meV (cf. Refs. [21, 22]). These numbers are important when one tries to understand why putting the total change $\Delta E_0^{tot}$ into the calculations of $g$ value, one obtains very different results in the two cases.

Finally, we consider average values of the spin $g$ factor measured as a function of temperature. The measurements are usually done in relatively pure samples having low free electron densities. The electrons are excited across the gap into the conduction band and into both spin states. The spin states are equally populated, but the circularly polarized light produces a well defined coherence between them. The excited electrons quickly thermalize and are distributed among LLs according to the lattice temperature without losing their spin or phase. Then they interfere and quantum beats in the photoluminescence or other effects are observed from many LLs. According to this picture the observed signal represents an average over the populated LLs in which the electron thermal distribution over LLs determines their contribution to the average $g$ value. This explains why various experiments performed on weakly doped samples give basically the same results depending only on the temperature.

We assume that the electron energies are

$$E_{nk_z}^\pm = \varepsilon_n^\pm + \frac{\hbar^2 k^2}{2m_0^*}, \quad (2)$$

where $n$ is the LL number, $\pm$ signs correspond to the two spin states, $k_z$ is the wavevector along the direction of $B$, and $m_0^*$ is the effective mass at the band edge. The energies $\varepsilon_n^\pm$ contain the intricacies of the band structure mentioned above, but we first assume a simple parabolic dependence on $k_z$ to make the averaging tractable. The spin $g$ value is defined as (in formulas we use $g^*$ symbol)

$$g^* = (E_{nk_z}^+ - E_{nk_z}^-)/\mu_B B. \quad (3)$$

An averaging procedure involves summation over $n$ and integrations over $k_x$ and $k_z$. A simple calculation gives the average value of $g^*$ in the form

$$\overline{g^*}(T) = \frac{A}{C}, \quad (4)$$
where

\[ A = \sum_{n=0}^{\infty} \int_{E_n}^{\infty} \frac{g_n^*(E)f(E, \zeta)}{(E - E_n)^{1/2}} dE, \quad (5) \]

and

\[ C = \sum_{n=0}^{\infty} \int_{E_n}^{\infty} \frac{f(E, \zeta)}{(E - E_n)^{1/2}} dE, \quad (6) \]

in which the summation is over the LLs, \( f(E, \zeta) \) is the Fermi-Dirac distribution function, and the square roots come from the integrations over \( k_z \). The integrations begin from the lower states \( E_n \) for each \( n \), which can be either \( E_n^+ \) or \( E_n^- \).

The average \( g \) value, as given by Eq. (4), is affected by the temperature in two opposite ways. According to the five-level model the spin \( g \) value at the conduction band edge is [10],

\[ g_0^* = 2 + \frac{2}{3} \left[ E_{P_0} \left( \frac{1}{E_0} - \frac{1}{G_0} \right) + E_{P_1} \left( \frac{1}{G_1} - \frac{1}{E_1} \right) \right] + \frac{4\Delta^2}{E_{P_0}E_{P_1}} \left( \frac{2}{E_1G_0} + \frac{1}{E_0G_1} \right) + 2C, \quad (7) \]

where \( E_{P_0} = 2m_0P_0^2/\hbar^2 \), \( E_{P_1} = 2m_0P_1^2/\hbar^2 \), \( G_0 = E_0 + \Delta_0 \) and \( G_1 = E_1 + \Delta_1 \). The spin-orbit energies \( \Delta_0 \) and \( \Delta_1 \) relate to \( (\Gamma_7^x, \Gamma_8^x) \) and \( (\Gamma_7^y, \Gamma_8^y) \) levels, respectively. \( \Delta \) is the interband matrix element of the spin orbit interaction between the \( (\Gamma_7^x, \Gamma_8^x) \) and \( (\Gamma_7^y, \Gamma_8^y) \) multiplets (see [10, 22]), and \( C \) is due to far-band contributions. For \( \Delta = 0 \) Eq. (7) reduces to the formula given first by Hermann and Weisbuch [23].

It follows from Eq. (7) that, as the temperature \( T \) increases and the absolute value of the fundamental gap \( E_0 \) decreases (see Fig. 2), the spin \( g_0^* \) value at the band edge decreases. On the other hand, with increasing \( T \) the electrons populate higher LLs and band’s nonparabolicity comes more and more into play. The latter is known to make the \( g \) value less negative (see Refs. [10, 24], and Fig. 3). Thus, as \( T \) increases, the average \( g^* \) decreases or increases depending on the relative strength of the two effects. It is now clear why putting into calculations only the dilatational part of the gap variation makes the first effect weaker, i.e. it favors increase of the \( g \) values. We emphasize that we do not use in our calculations Eq. (7), it is quoted only to make clear the dependence of \( g_0^* \) on \( E_0 \). Calculating the electron energies away from the band edge we deal with the effects of band’s nonparabolicity and inversion asymmetry, as explained above. We use the following band parameters of GaAs at \( T = 0 \): \( E_{P_0} = 27.865 \) eV, \( E_{P_1} = 2.361 \) eV, \( E_0 = -1.519 \) eV, \( G_0 = -1.86 \) eV, \( E_1 = 2.969 \) eV, \( G_1 = 3.14 \) eV, \( C = -2.3107 \), \( C' = -0.0375 \). The zero of energy is chosen at the conduction band edge. The above values are the same as those established by an overall fit of various experiments on GaAs (see Ref. [10]) with the exception of the far-band contribution \( C' \), as discussed below. It is assumed that only \( E_0 \) depends on the temperature, see discussion below.

In Fig. 3 we plot the \( g \) values for consecutive LLs at two temperatures, as determined from definition (3), in which the energies are calculated for \( B = 4 \) T using the procedure described above. It is seen that, for a given temperature, as the energy increases with the growing Landau number \( n \), the \( g \) factor increases due to band’s nonparabolicity. On the other hand, for a given LL the \( g \) factor decreases with increasing temperature. The number of points for a given temperature indicates how many LLs are involved in the averaging, for still higher LLs the occupation by electrons is so small that their contribution is negligible. It should be noted that the \( g \) factors shown in Fig. 3 do not saturate at high energies at the free electron value of +2, as predicted by simple versions of the three-level or five-level \( k\cdot p \) models (see e.g. [24]). The reason is that our present theory includes the bulk inversion asymmetry (also called the Dresselhaus effect), which is manifested by the appearance of the matrix element \( Q \). Also, the increase of \( g \) factor with the energy, as shown in Fig. 3, is stronger than linear, whereas the one shown in Fig. 8 of Ref. [10] is weaker than linear. This is caused by the fact that in Fig. 3 the energy increases by going to high LLs (at constant \( B \)), whereas in Ref. [10] the energy is increased by going to high magnetic fields (at \( n = 0 \)).

III. RESULTS AND DISCUSSION

Fig. 4 shows the temperature dependent \( g \) values of electrons extracted from time-resolved Faraday rotation measurements performed at \( B = 4 \) T on undoped bulk GaAs (full squares). In addition, data taken from the literature and our calculations are shown. As to the experiments, the previously published data obtained with the use of time-resolved photoluminescence [1-3] and time-resolved Kerr rotation [25] are compared with our present results obtained by the time-resolved Faraday rotation. All these time-resolved experiments measure the phase coherence of spin states excited by circularly polarized light in the Voigt geometry and differ mostly in its detection. It is seen that the obtained data agree well with each other and all show an almost linear increase of \( g \) with the temperature. However, there is some discrepancy between various measured \( g \) values at \( T = 0 \), cf. [23, 26, 27]. Since all the \( g \) values presented in Fig. 4 were measured at magnetic fields \( B \) of a few Tesla, they should be higher than the band edge value \( g_0^* \) since they are affected by band’s nonparabolicity. In this situation we take the value of the far-band contributions \( C' \), as given above, to give our measured value of \( g^* = -0.452 \) at \( T = 0 \) and \( B = 4 \) T. This corresponds to the band edge value \( g_0^* = -0.472 \). Preference to a different experimental band edge \( g \) value would simply require a slightly different \( C' \).
is important that the improved experiment and theory exhibit this property.

Coming to the discussion of our results, one should keep in mind that our theoretical description, although representing a considerable improvement over the procedure of Ref. [4], is still approximate. The reason is that we made an assumption about the $k_z$ dependence of the $g$ factor. This assumption is reasonable and it allows us to calculate the $E_n^\pm$ energies and carry out the averaging procedure over LLs in a relatively simple way. Still, in principle one should include the $k_z$ terms from the beginning in the computation procedure, calculate the $k_z$ dependence of different LLs and carry out a numerical summation over $k_z$ values. This, however, makes the problem difficult for two reasons. First, if the $k_z$ terms are included, one must take much larger truncated determinants to obtain convergent values of $E_n^\pm(k_z)$ energies. Second, when performing the averaging procedure one must integrate numerically over $k_z$ for each LL separately since in principle each LL has a different $k_z$ dependence. Our simplifying assumption allowed us to get around the above difficulties.

As to the work of other authors, Oestreich and Ruhle [1] put into the theoretical description the total temperature change of the energy gap but neglected band’s nonparabolicity. Such a description predicted a decrease of the $g$ factor with temperature which contradicted the experimental results. Oestreich et al [2] and Huebner et al [3] included in their description band’s nonparabolicity but neglected important features of the band structure: the interband matrix element of momentum $Q$ and of the spin orbit interaction $\Delta$ between the $(\Gamma_7^v, \Gamma_6^v)$ and $(\Gamma_5^v, \Gamma_8^v)$ multiplets. Both these quantities have an important influence on the $g$ value, which we illustrate numerically. Using our band parameters and $\Delta \neq 0$ the band edge $g$ value is $g_0^0 = -0.472$, while for the same parameters and $\Delta = 0$ there is $g_0^0 = -0.346$ (see Eq. (7)). The element $Q$ does not enter the conduction band edge quantities, but at $T = 300$ K and $B = 4$ T our calculated average value of $g$ including $Q$ is $\bar{g}(T) = -0.297$, while for $Q = 0$ the calculated average is $\bar{g} = -0.396$. Also, Refs. [2], [3] did not include the Landau quantization of the conduction band, so that the calculated average $g$ value did not depend on the magnetic field intensity. Finally, and this is the decisive point, it was assumed that the $g$ value depends on the temperature via the total (i.e. measured) change of the fundamental gap, whereas one should take the change due to thermal lattice dilatation alone. When this is done, there is no need to introduce a temperature variation of the interband matrix element of momentum $P_0$, as was done in Ref. [3]. Consideration of the momentum operator and of the wave functions indicates that the interband momentum matrix element should also scale with the lattice dilatation, its square should change no more than 0.1 % in the temperature range from 0 to $300$ K, so it can be neglected [4].

The latest analysis by Litvinenko et al [4], including the matrix elements $\Delta$ and $Q$ and the band nonparabolic-
ity on one side and taking only the dilatation contribution to the change of the energy gap on the other, was able to account for the first time for the experimental increase of the spin $g$ factor with the temperature. However, this analysis assumed no $k_z$ dependence of the Landau levels and, consistently, took the average electron energy for the Boltzmann statistics to be equal to $kT$. This corresponds roughly to our dashed curve in Fig. 4, which assumes no dependence of $g$ on $k_z$. If one includes the $k_z$ dependence of the energy, the average nondegenerate electron energy is $\bar{E} = (3/2)kT$ which, upon using Fig. 3 for $g_0(\bar{E})$, corresponds quite well to the solid line in Fig. 4. In other words, if one applies a proper averaging procedure to the $g$ value, the resulting $g^\ast(T)$ corresponds quite well to averaging the electron energy $\bar{E}$ and taking $g^\ast(\bar{E})$. One should add that, taking the thermal change of gap due to the dilatation alone, Litvinenko et al [4] were able to account correctly for the temperature dependence of the electron spin splitting in InSb. All this, together with the published analysis of $m^\ast(T)$ in GaAs [14, 15], strongly confirms that both orbital and spin quantizations of the electron spectrum in a magnetic field are governed by the change of the energy gap due to lattice dilatation alone.

**IV. SUMMARY**

We investigated experimentally and theoretically the controversial problem of temperature dependence of the spin $g$ factor in GaAs. The time-resolved Faraday rotation technique was used to show that, in agreement with other data, the $g$ factor increases almost linearly with $T$ up to room temperature. This increase is successfully described by the five-level $\mathbf{k}\cdot\mathbf{p}$ model of the band structure for GaAs. As the temperature increases there occur two effects having an opposite influence on the $g$ value. On one hand, a decrease of the fundamental energy gap caused by the thermal lattice dilatation leads to a decrease of $g$. On the other hand, at higher temperatures electrons populate higher Landau levels which, due to band’s nonparabolicity, leads to an increase of the average $g^\ast(T)$ value. A very good agreement of our theory with the experimental increase of $\bar{g}(T)$ indicates that the band nonparabolicity effect dominates. Our interpretation confirms the validity of the complete five-level $\mathbf{k}\cdot\mathbf{p}$ model for the conduction band of GaAs.

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