Principal thermodynamic properties of quasi-two-dimensional carriers under in-plane magnetic field

2009 J. Phys.: Condens. Matter 21 015304

(http://iopscience.iop.org/0953-8984/21/1/015304)

J. Phys.: Condens. Matter **21** (2009) 015304 (6pp) doi:10.1088/0953-8984/21/1/015304

Principal thermodynamic properties of quasi-two-dimensional carriers under in-plane magnetic field

Constantinos Simserides

Institute of Materials Science, National Center of Scientific Research Demokritos, GR-15310 Athens, Greece

E-mail: simserides@ims.demokritos.gr

Received 13 August 2008, in final form 2 November 2008
Published 2 December 2008
Online at stacks.iop.org/JPhysCM/21/015304

Abstract

An external magnetic field, H, applied parallel to a quasi-two-dimensional carrier system modifies quantitatively and qualitatively the density of states. We examine how this affects primary thermodynamic properties, namely, the entropy, S, the internal and free energy, U and F, the magnetization, M, and the magnetic susceptibility, χ_m, using a self-consistent numerical approach. Although M is mainly in the opposite direction to H, the system is not linear. Hence, surprisingly, $\partial M/\partial H$ swings between negative and positive values, i.e. a diamagnetic to paramagnetic transition of entirely orbital origin is predicted. This phenomenon is important compared to the ideal de Haas–van Alphen effect, i.e. the corresponding phenomenon under perpendicular magnetic field. By augmenting temperature, the diamagnetic to paramagnetic transition fades away. The overall behaviour of entropy is also foreseen and consistently interpreted. While the entropy contribution to the free energy is very small at low temperatures, entropy shows a clear dependence on the external magnetic field.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The study of quasi-two-dimensional (2D)[1] carriers under magnetic field has a long, fruitful history. Emphasis has been given to the configuration where the magnetic field, H, is applied perpendicularly to the quasi-2D system, leading to quantization of the free in-plane motion into Landau levels [1]. In this configuration the integer quantum Hall effect [2] was discovered and the fractional quantum Hall effect was observed [3] and explained in terms of quasiparticles with fractional charge [4]. Besides varying H, oscillations of the conductivity (the Shubnikov–de Haas effect [5]) as well as oscillations of the magnetic susceptibility (the de Haas–van Alphen effect) were observed. The de Haas–van Alphen effect, involving measurements of a thermodynamic property like the magnetization, M, directly probes the heart of the system, i.e. the density of states (DOS). However, experimental evidence of the ideal de Haas–van Alphen effect in a quasi-2D carrier system was only found recently by Wilde *et al* [6] who measured the magnetization oscillations of *high mobility* electrons in modulation-doped AlGaAs/GaAs heterostructures. In the sample with the highest oscillation amplitude they observed discontinuous jumps in M with peak-to-peak amplitude of two effective Bohr magnetons[2] per electron, in agreement with the old Peierls prediction [7]. Numerical simulations [6] assuming no states between the Landau levels (no 'background' DOS) could model these jumps quantitatively, but measurements on samples with lower mobility revealed a finite background DOS. Indeed in earlier studies [8] a considerable DOS between the broadened Landau levels was necessary to simulate the experimental results.

This paper predicts how the DOS modification—caused by a magnetic field *parallel* to a quasi-2D system—amends fundamental thermodynamic properties, namely, the entropy, the internal and the free energy, the magnetization, and the magnetic susceptibility. A fully self-consistent numerical

[1] The most popular term is 'two-dimensional', e.g. two-dimensional electron gas (2DEG). Strictly speaking, 'quasi-two-dimensional' is more appropriate because there is a finite extension in the third direction.

[2] $\mu_B^* = \frac{e\hbar}{2m^*}$, m^* is the effective mass.

envelope function approach is employed. Although M remains basically in the opposite direction to H, the system is highly nonlinear. As a result, the magnetic susceptibility oscillates between negative and positive values. This is the first prediction of a purely orbital diamagnetic to paramagnetic transition. The effect, ignored by the community up to now, is important compared to the ideal de Haas–van Alphen effect, the analogous phenomenon under perpendicular magnetic field. This work will hopefully also help the interpretation of magnetization measurements under tilted H, i.e. whenever an in-plane component of H exists. In addition, the overall behaviour of entropy and in particular its minimum and maximum, is consistently explained for the first time.

Basic theory is laid out in section 2. In section 3 we discuss low-temperature results, while in section 4 we increase temperature. In section 5 we state our conclusions.

2. Theory

When a quasi-2D system is subjected to an in-plane-or even tilted magnetic field, the charming concept of Landau levels must be *revised*, because carriers move under the competing influence of the Lorentz force and the force due to the quantum well (QW) confining potential. The equal-energy surfaces [9] or equivalently the density of states [10, 11] are qualitatively and quantitatively modified because the spatial and the magnetic confinement compete. Generally, a proper treatment involves self-consistent computation [9, 11, 12] of the energy dispersion, $E_{i,\sigma}(k_x)$. i is the subband index, σ denotes the spin, and k_x is the in-plane wavevector perpendicular to the external in-plane magnetic field (applied along y), H. The envelope functions along the 'growth' z-axis depend on k_x i.e. $\psi_{i,\sigma,k_x,k_y}(\mathbf{r}) \propto \zeta_{i,\sigma,k_x}(z)\mathrm{e}^{\mathrm{i}k_x x}\mathrm{e}^{\mathrm{i}k_y y}$. The consequences of this modification were initially realized in transport [13] experiments. This change influences the character of plasmons [14]. The $\mathcal{N}$-type kink was predicted [15] and recently verified in photoluminescence experiments [16]. The impact of the DOS modification on the properties of dilute-magnetic-semiconductor single QWs was studied recently [12, 17]. A Monte Carlo study of transport properties appeared [18], too. Thus, it seems that the parallel or tilted configuration offers new avenues to explore. A compact DOS formula for a quasi-2D system under in-plane H, valid for any kind of interplay between spatial and magnetic confinement, exists [12]:

$$\rho(\mathcal{E}) = \frac{A\sqrt{2m^*}}{4\pi^2\hbar}\sum_{i,\sigma}\int_{-\infty}^{+\infty} \mathrm{d}k_x \frac{\Theta(\mathcal{E} - E_{i,\sigma}(k_x))}{\sqrt{\mathcal{E} - E_{i,\sigma}(k_x)}}. \quad (1)$$

The QWs are along the z-axis. H is applied along the y-axis. Θ is the step function, A is the xy-area of the structure. Generally the spin-dependent xz-plane eigenenergies, $E_{i,\sigma}(k_x)$, must be self-consistently calculated [9, 11, 12, 15, 17]. The k_x dependence in equation (1) often increases the numerical cost by a factor of 10^2–10^3; hence it is sometimes overlooked, but this is only justified for narrow single QWs or for $H \to 0$. With the existing computers, such a compromise is not needed. For $H \to 0$, equation (1) converges to the staircase form with the famous step $\frac{1}{2}\frac{m^* A}{\pi\hbar^2}$ for each spin. In the opposite asymptotic limit of equation (1), at a simple saddle point, the DOS diverges logarithmically [10]. The DOS modification drastically affects the physical properties [9–17]; models which ignore it can only be applied to narrow single QWs or for $H \to 0$. For completeness, we note that in equation (1) disorder is ignored; with the progress of epitaxial techniques, it is fairly small in well-prepared III–V structures. Disorder will induce some broadening of the subbands.

The population, N, the internal energy, U, the entropy [19], S, and the free energy, F, are given by:

$$N = \int_{-\infty}^{+\infty} \mathrm{d}\mathcal{E}\, \rho(\mathcal{E}) f_0(\mathcal{E}), \quad (2)$$

$$U = \int_{-\infty}^{+\infty} \mathrm{d}\mathcal{E} \rho(\mathcal{E}) f_0(\mathcal{E})\mathcal{E}, \quad (3)$$

$$S = -k_{\mathrm{B}} \int_{-\infty}^{+\infty} \mathrm{d}\mathcal{E} \rho(\mathcal{E}) f_0(\mathcal{E}) \ln[f_0(\mathcal{E})], \quad (4)$$

$$F = U - TS. \quad (5)$$

T is the temperature. $f_0(\mathcal{E})$ is the Fermi–Dirac distribution function. $\rho(\mathcal{E}) \propto A$, thus N, U, S as well as F are proportional to A. However, the magnetization,

$$M = -\frac{1}{V}\left(\frac{\partial F}{\partial B}\right)_{N,T}, \quad (6)$$

where V is the structure's volume, is independent of A. To have units in Tesla, we symbolize $B = \mu_0 H$, μ_0 as being the magnetic permeability of free space. To calculate M we have to keep T as well as N constant e.g. assuming all dopants are ionized. In section 3, $T = 4.2$ K, while in section 4, the temperature dependence of the thermodynamic quantities is examined. N_i are the sheet subband concentrations and $N_{\mathrm{s}} = N/A$ is the sheet concentration. We use $E_i(k_x)$ for the subband energy dispersion, i.e. in the present work we ignore spin-splitting which has been treated in detail elsewhere [17]. For $H = 0$, the symmetric–asymmetric gap $\Delta SAS = E_1(k_x = 0) - E_0(k_x = 0)$.

3. Low-temperature results and discussion

The phenomena described below apply to all quasi-2D systems. As a prototype system, we choose GaAs/(Al,Ga)As double QWs, a bilayer system with well-defined ΔSAS and well-known material parameters. Magnetization measurements under perpendicular H of a similar system can be found elsewhere [20]. To facilitate the reader, we provide in figure 1 the self-consistent potential energy profiles, for $H = 0$, of the various double QWs employed here. These include the Coulomb term obtained by the solution of the 'Poisson' equation, the term due to the discontinuity of the conduction band minimum as well as the exchange and correlation term [11]. These terms are also included when H is switched on. Two (left and right) 50 nm spacers separate the δ-doped layers from the double QW. The total double QW width is 22.7 nm, including the internal barrier of 2.5 nm. Augmenting the δ-doping, we vary

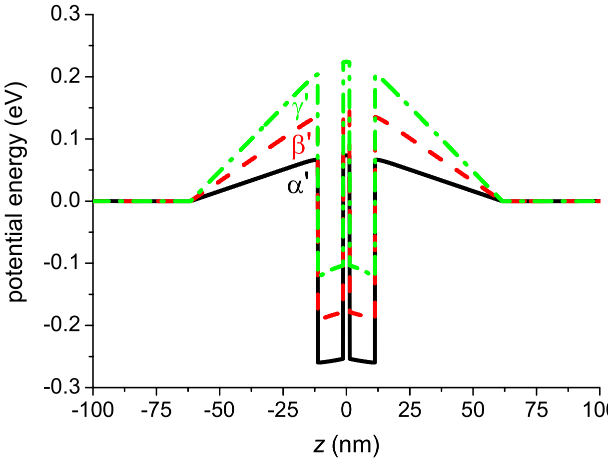

Figure 1. Quantum well potential energy profiles for $H = 0$. (α') $N_s = 1.85 \times 10^{11}$ cm^{-2}, $\Delta SAS = 4.24$ meV. (β')$N_s = 3.70 \times 10^{11}$ cm^{-2}, $\Delta SAS = 4.01$ meV. (γ')$N_s = 5.55 \times 10^{11}$ cm^{-2}, $\Delta SAS = 3.79$ meV. $T = 4.2$ K.

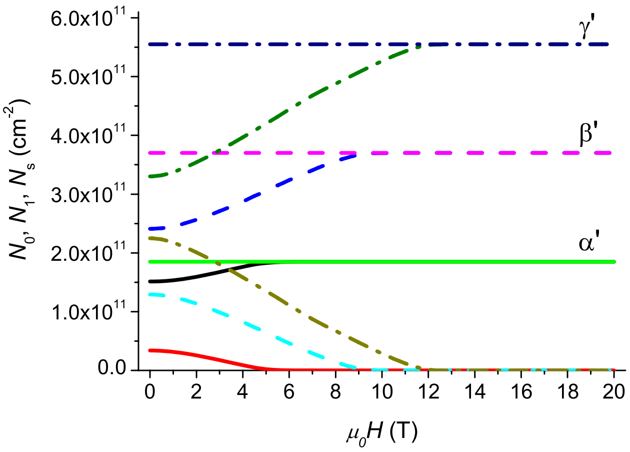

Figure 2. The sheet subband concentrations N_0, N_1 and the sheet concentration N_s as functions of the external in-plane magnetic field, $\mu_0 H$, for cases α' (solid lines), β' (dashed lines), γ' (dash–dotted lines). $T = 4.2$ K.

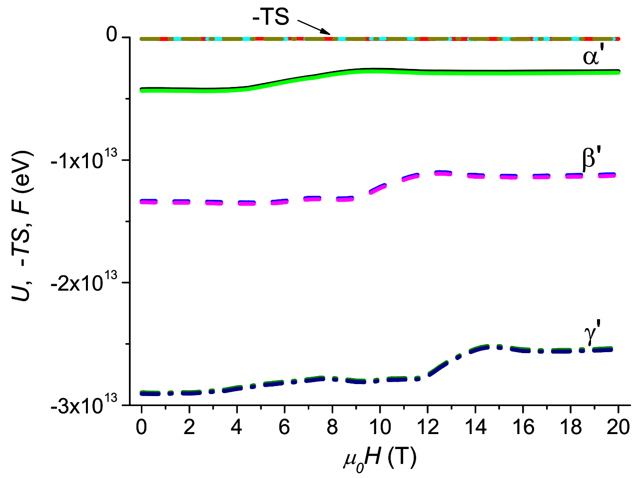

Figure 3. The internal energy, U, the product $-TS$, and the free energy, F, as functions of the external in-plane magnetic field, $\mu_0 H$, for all cases (α', β', γ'). On this scale, $F \approx U$, $-TS$ is negligible. $T = 4.2$ K.

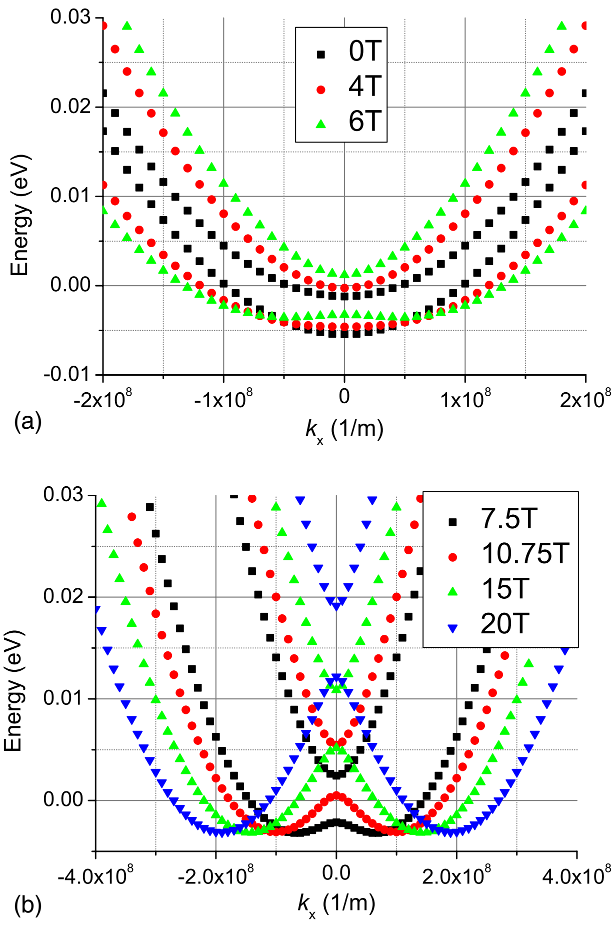

Figure 4. Enlarged views of the energy dispersion, $E_i(k_x)$ ($i = 0, 1$), for characteristic values of $\mu_0 H$, for case (α'). Here the Fermi energy, E_F, is identified with zero. $T = 4.2$ K.

N_i, N_s, and ΔSAS, distinguishing three cases (α', β', γ') with $N_s(\alpha')$:$N_s(\beta')$:$N_s(\gamma') = 1$:2:3. Figure 2 depicts N_0, N_1 and N_s as functions of $\mu_0 H$. The depopulation of E_1 induced by the DOS modification occurs approximately at 6, 10, and 12.5 T, respectively.

Figure 3 depicts U, $-TS$, and F, as functions of $\mu_0 H$. For simplicity we take $A = 1$ m^2. At $T = 4.2$ K, $|F| \approx |U| \gg |-TS|$. Since N is kept constant in each case, we expect that $|U|$ will decrease whenever H induces 'flattening' of the occupied subbands i.e. expansion of the occupied parts to higher $|k_x|$, because this leads to occupied energies with smaller $|\mathcal{E}|$. The gradual increase of $|F|$ from (α') to (β') and (γ') mirrors the population increase. To facilitate the reader, we provide in figure 4 enlargements of the energy dispersion of case (α') for characteristic values of $\mu_0 H$.

Figure 5 depicts the entropy S as a function of $\mu_0 H$. From equations (2) and (4), since for each case N is constant, S is sensitive to the changes of $\ln[f_0(\mathcal{E})]$. At $T = 4.2$ K, these changes only occur in a short region around the Fermi energy, E_F. In other words, S *reads* the modification of the energy dispersion around E_F. For the case (α'), for $\mu_0 H = 0$, the

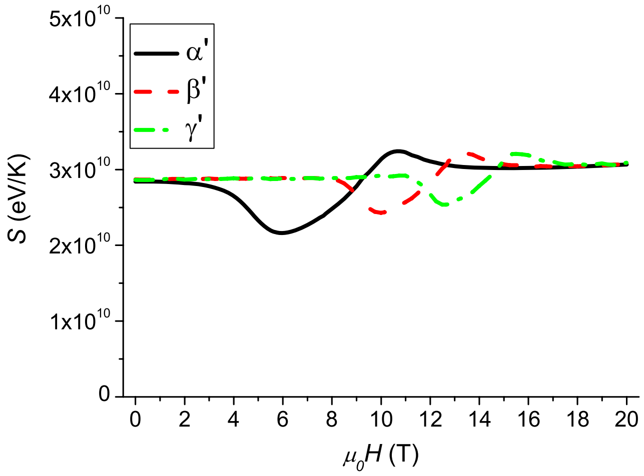

Figure 5. The entropy, S, as a function of $\mu_0 H$, for each one of the cases (α', β', γ'). $T = 4.2$ K.

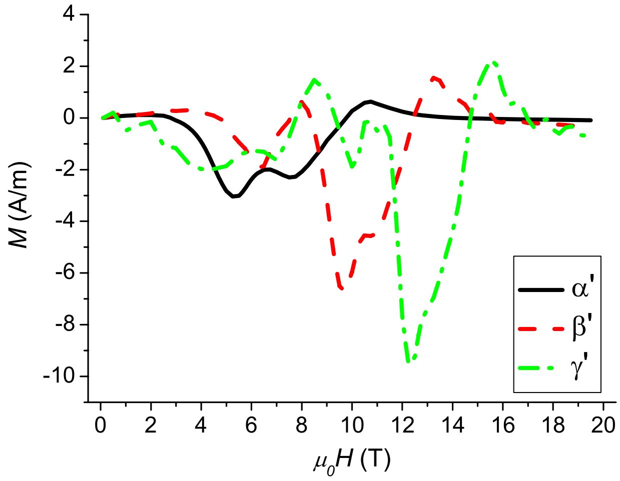

Figure 6. The magnetization, M, as a function of $\mu_0 H$, for each one of the cases (α', β', γ'). $T = 4.2$ K.

bottom of $E_1(k_x)$ is pretty close to E_F. From 0 to 6 T, S continuously falls due to the continuous depopulation process of $E_1(k_x)$. The minimum of S occurs at 6 T because there the gradual DOS modification completely depopulates the first excited subband, cf figures 2 and 4. In other words, the 'cohesion' of the system reaches its maximum at 6 T. From 6 to 10.75 T, S continuously increases because around E_F, $E_0(k_x)$ in the range $|k_x| \approx 0$ moves upward and finally the populated $E_0(k_x)$ is divided into two parts, cf figure 4. The maximum of S occurs at 10.75 T because there $E_0(k_x)$ splits completely into two occupied parts, around $k_x = 0$ the ground state subband ceases to be occupied. Thus, the cohesion of the occupied $E_0(k_x)$ is lost around 10.75 T. From 11 to 20 T, S does not change much, because the main effect of increasing $\mu_0 H$ is to move the two $E_0(k_x)$ minima continuously apart, cf figure 4. The behaviour of S, in cases (β', γ') can be readily explained likewise. As one could maybe imagine, increasing the system's magnitude, the minimum of entropy, $S_{\min}$, is increasing: at 6 T with $S_{\min} = 2.2 \times 10^{10}$ eV K^{-1}, at 10 T with $S_{\min} = 2.4 \times 10^{10}$ eV K^{-1}, at 12.5 T with $S_{\min} = 2.5 \times 10^{10}$ eV K^{-1}.

Figure 6 shows the magnetization M as a function of $\mu_0 H$. We observe that the DOS modification induces an oscillation of M; it is between ≈ -3 and ≈ 0.5 A m^{-1} for case (α'), between ≈ -7 and ≈ 2 A m^{-1} for case (β'), and between ≈ -9 and ≈ 2 A m^{-1} for case (γ'). The reader may observe that the magnetic susceptibility, $\chi_m = \partial M / \partial H$, swings between negative and positive values, thus figure 6 shows a totally *orbital* diamagnetic to paramagnetic transition. This is the first prediction of oscillations of the magnetic susceptibility under in-plane magnetic field. The new effect is important compared to the well-known de Haas–van Alphen effect (oscillations of the magnetic susceptibility under perpendicular magnetic field). For example in case (γ'), the fluctuation of M of the order of 10 A m^{-1} is translated to approximately $\frac{1}{5}$ of the ideal de Haas–van Alphen effect i.e. the magnetization step of two effective Bohr magnetons per electron in the perpendicular configuration [6, 7]. We hope that the new finding will be verified when magnetization experiments under purely in-plane magnetic field are carried out. The predicted effect will hopefully also help the interpretation of magnetization measurements under tilted H, i.e., whenever an in-plane component of H exists.

The self-consistent approach followed in the present manuscript can be applied not only to double quantum wells but also to narrow to wide single quantum wells, and for a wide range of magnetic fields, i.e. for any type of interplay between spatial and magnetic confinement. Hu and MacDonald [21] studied the magnetization of double quantum wells subject to (more general) tilted magnetic field. In this comprehensive paper the authors focused on the effect of the perpendicular component of the magnetic field. As far as the in-plane component of the magnetic field is concerned, they (i) took a narrow well approximation for each 2D layer and used a tight binding approximation so that the single-particle problem could be characterized by the interlayer distance d and the hopping integral t_0. In their approach, the dispersion relations for electrons in the separate layers remain quadratic but the minima are shifted along the k_y axis (this would be the k_x axis with the current choice of coordinates) in proportion to the in-plane magnetic field. This allowed them to write an analytical expression for the eigenenergies (equation (2.4) [21]). (ii) On the other hand, when they applied a tilted magnetic field, they kept the in-plane component in the range zero to 3 T. Points (i–ii) mean that in their case—as far as the in-plane magnetic field is concerned—the spatial confinement dominates. On the contrary, the self-consistent approach followed in the present manuscript holds for any type of interplay between spatial and magnetic confinement. Indeed, in the current manuscript, the oscillations of the magnetization occur for higher values of the magnetic field, i.e. when the magnetic confinement becomes a competitive player in this game. Accordingly, the energy dispersion is not parabolic any more or equivalently the density of states deviates from the ideal step-like form both quantitatively and qualitatively (equation (1)). This way, in the general case, the energy eigenvalues cannot be expressed analytically but have to be calculated self-consistently at the expense of computer time [11, 22].

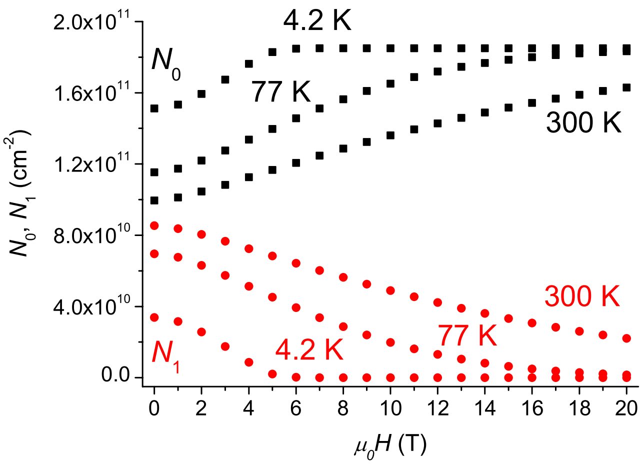

Figure 7. The sheet subband concentrations N_0, N_1 as functions of $\mu_0 H$, for $T = 4.2$, 77, and 300 K (case α').

4. Augmenting temperature

Let us examine the impact of increasing temperature. As an example, let us take case α'. Figure 7 presents the sheet subband concentrations N_0 and N_1 as functions of $\mu_0 H$ in steps of 1 T, for three characteristic temperatures, namely, 4.2, 77, and 300 K. As one could possibly imagine, the depopulation of the first excited subband, induced by the DOS modification caused by increasing $\mu_0 H$, becomes more difficult at higher temperatures.

Increasing T, the evolution of the internal energy U, the entropy S, the product $-TS$, and the free energy F as functions of $\mu_0 H$ in steps of 1 T, is summed up in figure 8. Not only $U_{300\ \mathrm{K}} > U_{77\ \mathrm{K}} > U_{4.2\ \mathrm{K}}$, but also $S_{300\ \mathrm{K}} > S_{77\ \mathrm{K}} > S_{4.2\ \mathrm{K}}$. We observe that at higher T, the contributions of U and of $-TS$ to F counterbalance in such a way that the oscillation of F as a function of $\mu_0 H$ fades away. Hence, with increasing T, the diamagnetic to paramagnetic transition dies out.

5. Conclusion

This paper examined principal thermodynamic quantities of quasi-2D carriers under parallel magnetic field. Magnetization measurements are a promising tool for the DOS investigation. We found that the DOS modification caused by the in-plane magnetic field generates a considerable effect in the magnetization of quasi-2D carriers which has been ignored by the community up to now. The magnetic susceptibility swings from negative to positive values, i.e. we have proved that an entirely *orbital* diamagnetic to paramagnetic transition exists. We conjecture that the in-plane component of a tilted magnetic field will bring about similar effects, hence care must be taken with the interpretation of such magnetization measurements. Many-body effects or the 'background' DOS may play their role, but we must not forget this major orbital effect stemming from essential quantum mechanics, i.e. from the k_x-dependence of the z-axis envelope functions. Additionally, it has been explained why the diamagnetic to paramagnetic transition dies out at higher temperatures. The

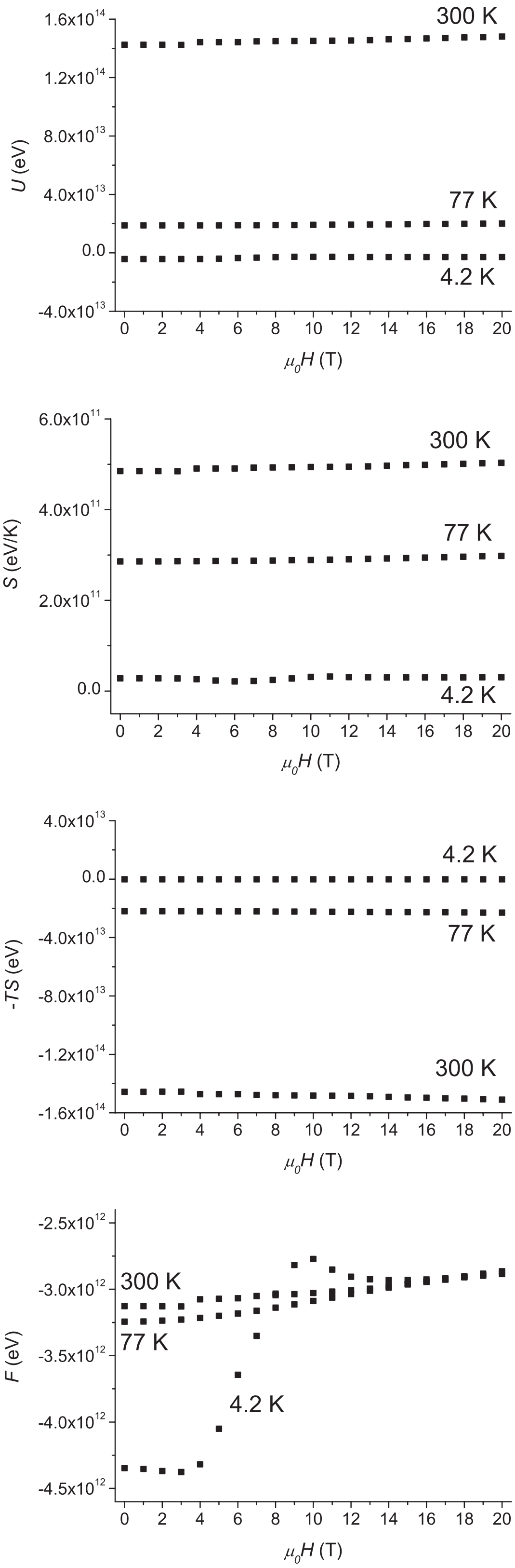

Figure 8. The internal energy U, the entropy S, the product $-TS$ and the free energy F as functions of $\mu_0 H$, for $T = 4.2$, 77, and 300 K (case α').

entropy was also calculated and interpreted, in particular the occurrences of its minimum and maximum were predicted. It was demonstrated that although the entropy contribution to the free energy is very small at low temperatures, entropy shows a clear dependence on the energy dispersion modification induced by the external magnetic field.

References

[1] Landau L 1930 *Z. Phys.* **64** 629
[2] von Klitzing K, Dorda G and Pepper M 1980 *Phys. Rev. Lett.* **45** 494
[3] Tsui D C, Störmer H L and Gossard A C 1982 *Phys. Rev. Lett.* **48** 1559
[4] Laughlin R B 1983 *Phys. Rev. Lett.* **50** 1395
[5] Fowler A B, Fang F F, Howard W E and Stiles P J 1966 *Phys. Rev. Lett.* **16** 901
[6] Wilde M A, Schwarz M P, Heyn C, Heitmann D, Grundler D, Reuter D and Wieck A D 2006 *Phys. Rev.* B **73** 125325
[7] Peierls R 1933 *Z. Phys.* **81** 186
[8] Eisenstein J P, Störmer H L, Narayanamurti V, Cho A Y, Gossard A C and Tu C W 1985 *Phys. Rev. Lett.* **55** 875
Wiegers S A J, Specht M, Lévy L P, Simmons M Y, Ritchie D A, Cavanna A, Etienne B, Martinez G and Wyder P 1997 *Phys. Rev. Lett.* **79** 3238
Harris J G E, Knobel R, Maranowski K D, Gossard A C, Samarth N and Awschalom D D 2001 *Phys. Rev. Lett.* **86** 4644
Schwarz M P, Wilde M A, Groth S, Grundler D, Heyn C and Heitmann D 2002 *Phys. Rev.* B **65** 245315
Zhu M, Usher A, Matthews A J, Potts A, Elliott M, Herrenden-Harker W G, Ritchie D A and Simmons M Y 2003 *Phys. Rev.* B **67** 155329
Wilde M A, Rhode M, Heyn C, Heitmann D, Grundler D, Zeitler U, Schäffler F and Haug R J 2005 *Phys. Rev.* B **72** 165429
[9] Smrčka L and Jungwirth T 1994 *J. Phys.: Condens. Matter* **6** 55
[10] Lyo S K 1994 *Phys. Rev.* B **50** 4965
[11] Simserides C 1999 *J. Phys.: Condens. Matter* **11** 5131
[12] Simserides C 2004 *Phys. Rev.* B **69** 113302
[13] Simmons J A, Lyo S K, Harff N E and Klem J F 1994 *Phys. Rev. Lett.* **73** 2256
Kurobe A, Castleton I M, Linfield E H, Grimshaw M P, Brown K M, Ritchie D A, Pepper M and Jones G A C 1994 *Phys. Rev.* B **50** 4889
Lay T S, Ying X and Shayegan M 1995 *Phys. Rev.* B **52** R5511
Jungwirth T, Lay T S, Smrčka L and Shayegan M 1997 *Phys. Rev.* B **56** 1029
[14] Cheng S-J and Gerhardts R R 2002 *Phys. Rev.* B **65** 085307
Tovstonog S V and Bisti V E 2003 *JETP Lett.* **78** 722
[15] Huang D and Lyo S K 1999 *Phys. Rev.* B **59** 7600
[16] Orlita M, Grill R, Hlídek P, Zvára M, Döhler G H, Malzer S and Byszewski M 2005 *Phys. Rev.* B **72** 165314
[17] Simserides C 2007 *Phys. Rev.* B **75** 195344
Simserides C and Galanakis I 2008 *Proc. 17th Int. Conf. on the Electronic Properties of Two-Dimensional Systems (Genova, 2007)*; *Physica* E **40** 1214
[18] Guo X G and Cao J C 2007 *Phys. Rev.* B **76** 045306
[19] Shannon C E 1948 *Bell Syst. Tech. J.* **27** 379
[20] Bominaar-Silkens I M A, Zeitler U, Christianen P C M, Reuter D, Wieck A D and Maan J C 2006 *Physica* E **34** 191
[21] Hu J and MacDonald A H 1992 *Phys. Rev.* B **46** 12554
[22] Simserides C 2004 *Physica* E **21** 956