Paramagnetic-diamagnetic interplay in quantum dots for non-zero temperatures

Paramagnetic–diamagnetic interplay in quantum dots for non-zero temperatures

Yu P Krasny[1,5]**, N P Kovalenko**[2]**, U Krey**[3] **and L Jacak**[4]

[1] Department of Mathematics, University of Opole, 45-052 Opole, Poland
[2] Department of Physics, Odessa State University, 65026 Odessa, Ukraine
[3] Institute of Physics II, University of Regensburg, 93040 Regensburg, Germany
[4] Institute of Physics, Wroclaw University of Technology, 50-370 Wroclaw, Poland

E-mail: krasnyj@math.uni.opole.pl

Abstract
In the usual Fock and Darwin formalism with a parabolic potential characterized by the confining energy $\epsilon_0 = \hbar\omega_0 \approx 3.4$ meV, but including explicitly also the Zeeman coupling between spin and magnetic field, we study the combined orbital and spin magnetic properties of quantum dots in a two-dimensional electron gas with the parameters for GaAs, for $N = 1$ and $N \gg 1$ electrons on the dot.

For $N = 1$ the magnetization $M(T, B)$ consists of a paramagnetic spin contribution and a diamagnetic orbital contribution, which dominate in a non-trivial way at low temperatures and fields and at high temperatures and fields respectively.

For $N \gg 1$, where orbital and spin effects are intrinsically coupled in a subtle way and cannot be separated, we find in a simplified Hartree approximation that at $N = m^2$, i.e. for a half-filled last shell, $M(T, B, N)$ is parallel (antiparallel) to the magnetic field, if temperatures and fields are low enough (high enough), whereas for $N \neq m^2$ the magnetization oscillates with B and N as a T-dependent periodic function of the variable $x := \sqrt{N}eB/(2m^*c\omega_0)$, with T-independent period $\Delta x = 1$ (where $m^* = 0.067\,m_0$ is the small effective mass of GaAs, while m_0 is the electron mass).

Correspondingly, by an *adiabatic demagnetization process*, which need only be fast enough with respect to the slow *transient time* of the magnetic properties of the dot, the temperature of the dot diminishes or increases with decreasing magnetic field, and in some cases we obtain quite pronounced effects.

(Some figures in this article are in colour only in the electronic version; see `www.iop.org`)

[5] Author to whom any correspondence should be addressed.

1. Introduction

In addition to the *charge* degrees of freedom, the *spin* of the electrons in quantum dots will certainly play an important role in future magneto-electronic devices for classical or quantum computing, involving quantum dots ('artificial atoms') [1], although the spin degrees of freedom are usually neglected, since typically the *orbital* magnetism dominates in quantum dots, as is known, and as we will also see below. However, in this paper we look at the *magnetic* properties of quantum dots more in detail, including the 'atypical' spin degrees of freedom, to see whether in this way one may be led to some 'new physics'. Moreover, it is clear that for our purpose it is *not* the most elaborate many-body techniques that are important; simple approaches should suffice for drawing relevant conclusions. With this in mind, we concentrate below on the two cases $N = 1$ and $N \gg 1$, where N is the number of electrons in the dot.

In any case, solids with quantum dots (i.e. planar artificial atoms) placed in an external magnetic field $\vec{B}$ have to acquire an additional magnetic moment. If the dots do not interact, this moment is $N_D \vec{M}$, where $\vec{M}$ is defined as the mean magnetic moment of a single dot and N_D the number of dots. That is why the following calculations reduce to considering the behaviour of a *single* dot in thermodynamic equilibrium with the surroundings. In this case we can consider the magnetic field $\vec{B}$ acting on the electrons in the dot as being identical to the external field.

In the following we always assume that the field $\vec{B}$ is constant in space and is in the z-direction, whereas the electrons move in the (x, y) plane.

2. The case of $N = 1$

To begin with, we consider the simple case of a dot with one electron. In such a model, and in the usual effective-mass approximation, the motion of the electron is described by the Hamiltonian

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m^*}\nabla^2 + \frac{1}{2}m^*\omega^2 r^2 + \frac{\hbar\omega_c}{2}(\hat{l}_z + g^*\hat{S}_z) \tag{1}$$

where m^* is the effective mass of the electron ($=0.067\,m_0$ for GaAs, where m_0 is the electronic mass), ∇^2 is the Laplacian in two dimensions, $\hbar = h/(2\pi)$, with h Planck's constant, $\omega_c = |e|B/(m^*c)$ is the cyclotron frequency, $\omega^2 := \omega_0^2 + \omega_c^2/4$, where ω_0 is the parameter characterizing the strength of the parabolic potential, which essentially confines the electron to the dot. Finally, $\hat{l}_z = -\mathrm{i}(x\,\partial/\partial y - y\,\partial/\partial x)$, with integer eigenvalues m, is the (reduced) operator of the *orbital angular momentum*, while the corresponding (reduced) *spin momentum* $\hat{S}_z$ has the eigenvalues $\pm\frac{1}{2}$ (here 'reduced' means 'measured in units of $\hbar$'). Furthermore, in the following we use the 'effective Bohr magneton':

$$\mu_B^* := \frac{\hbar\omega_c}{2B} = \frac{\hbar|e|}{2m^*c}.$$

Also, $g^* := (m^*/m_0)g$ is the corresponding effective g-factor, where for the free electron one would have $m^* = m_0$ and $g = 2$, whereas for GaAs, we have $g \cong -0.44$, and (as already mentioned) $m^* \cong 0.067\,m_0$. Therefore, for GaAs, the quantity $|g^*|$ is $\ll 1$, whereas $\mu_B^* \gg \mu_B$.

The eigenfunctions of the Hamiltonian (1) have the following form [2]:

$$\psi(\vec{r}, \sigma) = \varphi_{n_+, n_-}(\vec{r})\chi_{s_z}(\sigma) \tag{2}$$

where $\chi_{s_z}(\sigma)$ are normalized eigenfunctions of the spin operator $\hat{S}_z$ with eigenvalue $s_z = \pm\frac{1}{2}$, while the coordinate wavefunction can be written as

$$\varphi_{n_+, n_-}(\vec{r}) = \frac{(\hat{a})^{n_+}(\hat{b})^{n_-}}{l_0\sqrt{2\pi n_+!n_-!}}\exp\left(\frac{-|x + \mathrm{i}y|^2}{2l_0^2}\right). \tag{3}$$

Here

$$\hat{a} := \frac{1}{2i}\left[\frac{x+iy}{l_0} - l_0\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\right]$$

$$\hat{b} := \frac{1}{2}\left[\frac{x-iy}{l_0} - l_0\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)\right]$$

with $l_0^2 = \hbar^2/(m^*\omega)$; $n_\pm = 0, 1, 2, \ldots$; $s_z = \pm\frac{1}{2}$.

The energy eigenvalues corresponding to these wavefunctions are

$$\epsilon_{n_+,n_-,s_z} = \epsilon_+\left(n_+ + \frac{1}{2}\right) + \epsilon_-\left(n_- + \frac{1}{2}\right) + g^*\frac{\hbar\omega_c}{2}s_z \tag{4}$$

with $\epsilon_\pm := \hbar\omega \pm \frac{1}{2}\hbar\omega_c$.

The partition function $Z(T, B)$ of the system can be easily calculated and is equal to

$$Z(T, B) = \sum_{n_+=0}^{\infty}\sum_{n_-=0}^{\infty}\sum_{s_z=-1/2}^{1/2}\exp\left(-\frac{\epsilon_{n_+,n_-,s_z}}{k_BT}\right)$$

$$= \cosh\left(\frac{g^*\hbar\omega_c}{4k_BT}\right)\left[\cosh\left(\frac{\hbar\omega}{k_BT}\right) - \cosh\left(\frac{\hbar\omega_c}{2k_BT}\right)\right]^{-1} \tag{5}$$

where k_B is the Boltzmann constant and T the 'Kelvin temperature'. All other characteristic thermodynamic quantities can be found from $Z(T, B)$ by means of known derivatives. For instance, the mean moment of a dot is [3]

$$M = k_BT\frac{1}{Z}\left(\frac{\partial Z}{\partial B}\right)_T. \tag{6}$$

Thus for $N = 1$, the free enthalpy $G(T, B) = -k_BT\ln Z(T, B)$, and the magnetization as well, can simply be separated into a 'paramagnetic' spin contribution, corresponding to the first factor on the r.h.s. of (5), and the usual diamagnetic 'orbital' contribution corresponding to the second factor in (5). Due to the smallness of g^*, the paramagnetic contribution is very small in GaAs. However, at low fields, for high enough temperatures the spin contribution dominates in any case, since a systematic Taylor expansion shows that the 'paramagnetic factor' is

$$Z_{\text{spin}} \cong 1 + \frac{(g^*)^2e^2B^2}{8(m^*)^2k_B^2T^2} + \cdots$$

(i.e. the correction is $\propto B^2/T^2$), whereas the 'orbital factor' is

$$Z_{\text{orbital}} \cong 1 - \frac{\hbar^4\omega_0^2\omega_c^2}{48k_B^4T^4} + \cdots$$

(i.e. here the correction is $\propto B^2/T^4$). Note that here we have explicitly used the B-dependence of $\omega = \sqrt{(\omega_0^2 + \omega_c^2/4)}$, which is sometimes 'approximated away' too early.

Of course we are more interested in the low-temperature behaviour: in any case, the magnetization $M(T, B)$ can be calculated for $N = 1$ completely generally from the following formula, with $\beta := (k_BT)^{-1}$, and with the characteristic energy $\epsilon_B \propto B$, i.e. $\epsilon_B := \hbar\omega_c/2$:

$$\frac{M(T, B)}{\mu_B^*} = \frac{g^*}{2}\tanh\left(\frac{g^*\epsilon_B\beta}{2}\right) - \frac{\sinh\left(\sqrt{\epsilon_0^2 + \epsilon_B^2}\beta\right)\epsilon_B/\sqrt{\epsilon_0^2 + \epsilon_B^2} - \sinh(\epsilon_B\beta)}{\cosh\left(\sqrt{\epsilon_0^2 + \epsilon_B^2}\beta\right) - \cosh(\epsilon_B\beta)}. \tag{7}$$

This formula can be evaluated in various limits; i.e. due to the smallness of g^* for GaAs, one can consider for example the limit $g^*\epsilon_B\beta/2 \ll 1$ while at the same time $\epsilon_B\beta \gg 1$

(i.e. $\hbar|e|B/(2k_BT) \gg k_BT$), which is somewhat strange, although not unreasonable, if one considers fields in the tesla range and temperatures in the millikelvin region.

In the following, we also consider *adiabatic* demagnetization or magnetization processes, i.e. where during the change of B and the ensuing measuring processes the *entropy* of the dot is kept constant. This only implies that the changes of the B-field, and the measuring processes considered, must be much faster than the thermal relaxation of the dot to the surroundings, which is not unreasonable, since with advanced techniques magnetic fields can at present be changed significantly in two picoseconds [4,5], whereas the thermal relaxation of the electronic state of a quantum dot can be much slower, i.e. by several orders of magnitude [6].

Now an adiabatic change ΔB leads to a corresponding change ΔT, which is given by the relation

$$\left(\frac{\mathrm{d}T}{\mathrm{d}B}\right)_S = -\frac{(\partial S/\partial B)_T}{(\partial S/\partial T)_B} = -\frac{T}{C_B}\left(\frac{\partial M}{\partial T}\right)_B = +\frac{\beta}{C_B}\left(\frac{\partial M}{\partial \beta}\right)_B. \tag{8}$$

Here we have used the well-known relations $\partial S/\partial B = \partial M/\partial T$ (which follows from $\mathrm{d}G = -M\,\mathrm{d}B - S\,\mathrm{d}T$) and $C_B = T\,\partial S/\partial T$ (the 'heat capacity of the dot' at constant B). So from $\partial M/\partial \beta$, i.e. from (7), knowing ΔB and C_B (which must be >0 and can be calculated from the formula $C_B(T, B) = k_B T\,\partial^2[T \ln Z(T, B)]/\partial T^2$), one can directly evaluate ΔT.

So at very low temperatures, i.e. if $|g^*|\epsilon_B\beta/2 \gg 1$ and—of course—$\epsilon_0\beta \gg 1$, one obtains with the relation $\tanh(x) \cong 1 - 2\mathrm{e}^{-2x} + \cdots$, valid asymptotically for $x \gg 1$:

$$\frac{\partial \tilde{M}}{\partial \beta} := \frac{1}{\mu_B^*}\frac{\partial M(TB)}{\partial \beta} \cong \epsilon_B[(g^*)^2\mathrm{e}^{-|g^*|\epsilon_B\beta} - 2\mathrm{e}^{-2\epsilon_0\beta}]. \tag{9}$$

But the heat capacity C_B should remain positive for finite T. So for GaAs, in a range of sufficiently low temperatures and sufficiently low fields, i.e. for temperatures T *below* (*above*) a value $T_0(B)$ given by

$$\exp\left[-\frac{2\epsilon_0 - |g^*|\epsilon_B}{k_B T_0(B)}\right] = \frac{(g^*)^2}{2}$$

adiabatic demagnetization ($\mathrm{d}B < 0$) leads to a *decrease* (*increase*) of T. If—on the other hand—we do *not* assume $|g^*|\epsilon_B\beta \gg 1$, but the opposite limit $|g^*|\epsilon_B\beta \ll 1$, then we obtain $\partial \tilde{M}/\partial \beta = \epsilon_B[(g^*)^2/4 - k_B T/\epsilon_0]$, leading to a similar conclusion, now with $k_B T_0(B) \cong \epsilon_0(g^*)^2/4$, not depending on B.

In figure 1, for various values of B, we plot the values of $\tilde{M}(T, B) := M(T, B)/\mu_B^*$ against the temperature T—ranging from 0 K to $\approx$0.008 K—and the magnetic induction B—ranging from 0 to 0.08 T; the characteristic line $T_0(B)$ separating positive and negative values of M is given by the third-lowest contour line from the right, which ends for $T_0 \to 0$ at a value $B_k \approx 0.048$ T, and for $B \to 0$ at a value $T_k \approx 0.008$ K.

These are the values for GaAs, calculated with $\epsilon_0 = 3.37$ meV. (The corresponding values for $\epsilon_0 = 7.5$ meV are: $T_k \approx 0.018$ K; $B_k \approx 0.1$ T—i.e. they scale roughly $\sim\epsilon_0$, as expected.)

In figure 2, the *adiabatic derivative* $(\mathrm{d}T/\mathrm{d}B)_S$ from equation (8) is plotted over B (T) ranging from 0 to 5 T (from 0 to 6 K) in a 3D representation with contour lines. The special contour line separating positive and negative values of $(\mathrm{d}T/\mathrm{d}B)_S$ hardly depends on B over an extremely wide range of B-values, and is clearly visible (it is the line vertically above the points with $T \approx 3$ K). In agreement with the 'third principal law of thermodynamics', the adiabatic derivative $(\mathrm{d}T/\mathrm{d}B)_S$ always vanishes for $T \to 0$, for all values of B. But one should note that according to figure 2 and figure 3, $(\mathrm{d}T/\mathrm{d}B)_S$ piles up to very high values in the region $1\,\mathrm{K} \lesssim T \lesssim 1.8\,\mathrm{K}$, for B-values $\lesssim$0.016 T: i.e., as seen in figure 3, in this 'sensitive region' one can easily obtain values of the adiabatic derivative between 100 and 500, and even larger values for temperatures around 1.5 K, if the external magnetic field is around 0.001 T. Note,
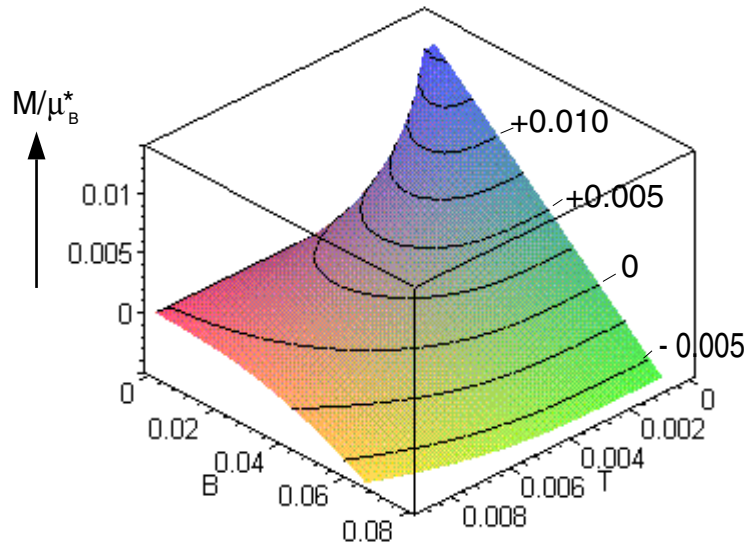
Figure 1. The reduced magnetization $M(T, B)/\mu_B^*$ is presented as a function of the temperature T (in K) and the magnetic induction B (in T) for a quantum dot with $N = 1$ electrons on it, in a two-dimensional electron gas with the parameters of GaAs, and with the confinement potential parameter $\epsilon_0 = \hbar\omega_0 = 3.37$ meV. Note the change of sign of M from paramagnetic behaviour ($M > 0$) to diamagnetic behaviour ($M < 0$) on crossing the contour line where $M(T, B) \equiv 0$. (The apparent discontinuities of the contour lines, representing $M(T, B)/\mu^* = -5 \times 10^{-3}, -2.5 \times 10^{-3}, \pm 0, +2.5 \times 10^{-3}, \ldots$, as indicated at the margin, are due to inaccuracies of the plotting software.)
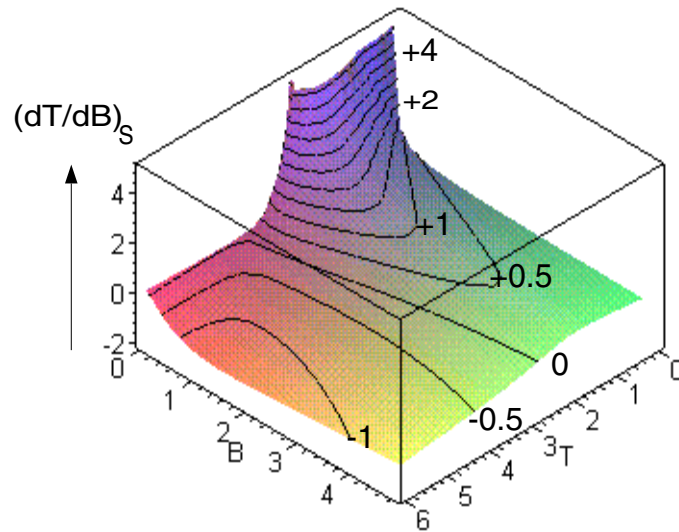

Figure 2. The 'adiabatic temperature derivative' $(dT/dB)_S$ is presented against the temperature T (in K) and the magnetic induction B (in T) for a quantum dot with $N = 1$ electrons on it, in a two-dimensional electron gas with the parameters of GaAs, and with the confinement potential parameter $\epsilon_0 = \hbar\omega_0 = 3.37$ meV. Note the change of sign of the derivative from positive values for low temperatures ($T < 3$ K) to negative values for higher temperatures, and note the strong increase in the region of 1.5 K for inductions below 1 T. (The apparent discontinuities of the contour lines $(dT/dB)_S(T, B) = -1, -0.5, \pm 0, +0.5, \ldots$, as indicated at the margin, are due to inaccuracies of the plotting software.)
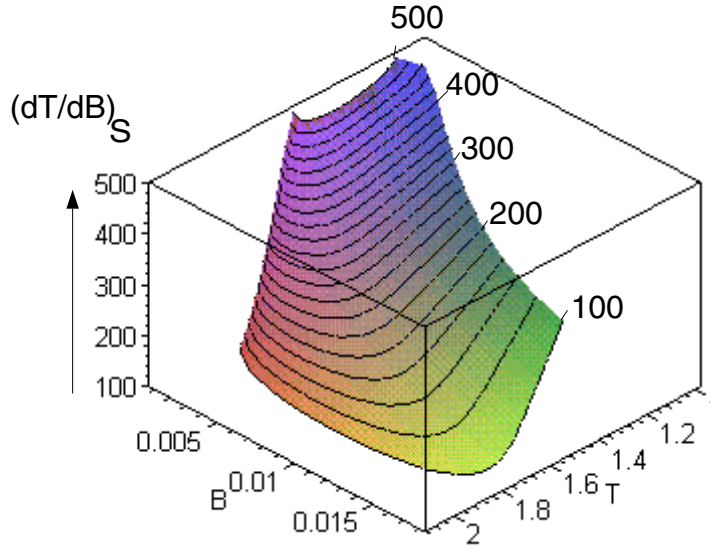
Figure 3. As figure 2, but for inductions as low as 0.002 T and below, where the 'adiabatic temperature derivative' reaches extremely high values. (The apparent discontinuities of the contour lines $(dT/dB)_S(T, B) = 100, 120, 140, \ldots$, as indicated at the margin, are due to inaccuracies of the plotting software.)

however, that in our theory we cannot consider naively the limit $B \to 0$, since the characteristic magnetic length, the 'cyclotron radius'

$$l_m(B) := \sqrt{\frac{\hbar}{m^* \omega_c}} = \sqrt{\frac{\hbar c}{eB}}$$

should be much smaller than the separation of two dots, or much smaller than any other geometrical extent of our 2D GaAs dot system (for $B = 1$ T, l_m is 25.7 nm). Keeping this constraint in mind, for change of the temperature by an infinitesimal adiabatic demagnetization in the above-mentioned 'sensitive region', we have the following result.

For an isolated quantum dot in 2D GaAs, with $N = 1$ electrons on the dot, starting at the point ($T \approx 1.5$ K, $B \approx 0.01$ T), for $\hbar\omega_0 \approx 3.37$ meV, we get $\Delta T/K \gtrsim 100\,\Delta B/T$. This implies that an unusually small adiabatic change of the magnetic field can lead to a significant change of the electron temperature in the dot, if one roughly hits the above-mentioned region.

Thus, on the one hand, we have the change of sign of the adiabatic derivative from positive values for $T < 3$ K to negative values for $T > 3$ K, a remarkable phenomenon in itself. On the other hand we have the fact that the change ΔT in the 'sensitive region' is also unusually large in magnitude, i.e. there it is really important to also explicitly consider the spin, and not only the orbital motion.

Therefore, to diminish the dot temperature (compared with that of the surrounding solid), e.g. by $\Delta T = -0.1$ K (at least for a transient time τ_T, which is determined by the small coupling of the dot to the degrees of freedom of the surrounding system, and which we assume to be much larger than the time τ_B necessary for significant changes ΔB of the magnetic field), in the above-mentioned region it is only necessary to decrease the magnetic field by $B \lesssim 10^{-3}$ T.

After having reached the thermodynamic equilibrium of the dot with its surroundings, its temperature increases again, but that of the solid decreases, until they equalize, i.e. the

final temperature has been lowered in any case. After that, the magnetic field can be turned off *isothermally* and the process can be periodically iterated. In such a way this process can be used for *magnetic cooling* of the dot system, which gives a flavour of the 'new physics' involved by controlling the magnetism of the dot.

All this will be considerably more effective—and also more interesting—for a large number of dots and for $N \gg 1$ electrons per dot.

3. The case $N \gg 1$—a simplified Hartree approach

3.1. Basic approximations

If the dot contains N electrons, the Hamiltonian is

$$\hat{\mathcal{H}} = \sum_{j=1}^{N} \left\{ -\frac{\hbar^2}{2m^*} \nabla_j^2 + \frac{1}{2} m^* \omega^2 r_j^2 + \frac{\hbar \omega_c}{2} (\hat{l}_{z,j} + g^* \hat{S}_{z,j}) \right\} + \frac{1}{2} \sum_{i,j}^{(\neq)} \frac{e^2}{\epsilon |\vec{r}_i - \vec{r}_j|}. \tag{10}$$

Here the inclusion of the Coulomb interaction for our multi-electron planar parabolic quantum dot leads to considerable complications in comparison to the case for free particles, since the Coulomb energy is of the same order of magnitude as the kinetic energy for electrons confined in dots. This Coulomb interaction is known to consist of the *direct* term (Hartree term) and the *exchange* term (Fock term): the former interaction is of long-range type, while the second one is short ranged (cf. [7, 8]) and oscillatory in its position dependence; cf. equation (13) in [9]. As a consequence, as shown in a long calculation in [10] for which we do not have a shorter argument, the ratio of the exchange energy divided by the Hartree energy decreases in $d = 2$ dimensions as $N^{-1/4}$. Therefore at sufficiently high N ($\gtrsim 10^2$–10^3) the exchange should no longer play the usual all-important central role—considering also exact calculations for $\mathcal{O}(10)$ electrons (see e.g. [9]), which show that then the above-mentioned ratio is $\lesssim 1/3$. So we neglect the exchange in a kind of zeroth-order approximation which still gives interesting analytical results for the B- and T-dependence (see below) generalizing directly those of the preceding section 2. (Including the exchange would preclude this analysis.)

Thus, from (10), we arrive at Hartree equations of the form [11]

$$\left\{ -\frac{\hbar^2}{2m^*} \nabla^2 + \frac{1}{2} m^* \omega^2 r^2 + \frac{\hbar \omega_c}{2} (\hat{l}_z + g^* \hat{S}_z) + V_j(\vec{r}) \right\} \psi_{p_j}(q) = \epsilon_{p_j} \psi_{p_j}(q) \tag{11}$$

where $q := (\vec{r}, \sigma)$; $j = 1, 2, \ldots, N$, and where the lower index p_j represents a triple of the *three* quantum numbers n_+, n_-, and s_z, and where $V_j(\vec{r})$ has to be determined self-consistently:

$$V_j(\vec{r}) := \frac{e^2}{\epsilon} \int d^2 r' \frac{n_j(\vec{r}')}{|\vec{r} - \vec{r}'|}$$

$$n_j(\vec{r}) := \sum_{i(\neq j)=1}^{N} \sum_{\sigma} |\psi_{p_i}(\vec{r}, \sigma)|^2.$$

ϵ is the dielectric constant of the solid, e.g. $\epsilon \approx 12.5$ for GaAs.

(Note that a numerical calculation supports the application of the Hartree approach, at least for the qualitative behaviour of multi-electron dots [12].)

For a solution of the Hartree equations we use as the zeroth approximation the semi-classical formula for $n(r)$ given in [13], i.e.

$$n_j(\vec{r}) \approx n(\vec{r}) = \begin{cases} \dfrac{3N}{2\pi R^2} \sqrt{1 - \dfrac{r^2}{R^2}} & \text{for } r \leqslant R \\ 0 & \text{otherwise.} \end{cases} \tag{12}$$

This approximate formula, which admittedly contradicts the boundary conditions for the harmonic oscillator functions, describes at least qualitatively the density of electrons inside the dot (comparison with exact numerical results for a small number of confined electrons [12, 14] shows that the quantum corrections to $n(r)$ do not modify it essentially except near the edge in cases of 'edge reconstruction', as discussed in the already mentioned paper [9]; see also chapter 4.7 in [2]).

As usual, for parabolic confinement we rely on the close connection between the 'effective dot radius R' used in (12) and the multi-electron wavefunction; therefore one can consider R also as the fitting parameter for this wavefunction.

In the zeroth order of perturbation we have with (12) for small r/R

$$V_j(r) \approx \frac{e^2}{\epsilon} \int \mathrm{d}^2 r' \, \frac{n(\vec{r}')}{|\vec{r} - \vec{r}'|} \approx \frac{3\pi N e^2}{4\epsilon R} \left(1 - \frac{r^2}{2R^2}\right). \tag{13}$$

As a consequence, in the interior of the dot (and not only there; see the remark below) we now get for the Hartree differential equation the simple 'renormalized form'

$$\left\{ -\frac{\hbar^2}{2m^*} \nabla^2 + \frac{1}{2} m^* \Omega^2 r^2 + \frac{\hbar \omega_c}{2} (\hat{l}_z + g^* \hat{S}_z) \right\} \psi_p(q) = E_p \psi_p(q) \tag{14}$$

i.e. through this equation we now have an *effective single-particle equation*, where the 'renormalized confining frequency' Ω, the 'renormalized single-particle energy' E_p, and the 'renormalized cyclotron length' l are defined as

$$\Omega^2 := \omega^2 - \frac{3\pi N e^2}{4\epsilon m^* R^3} \qquad E_p := \epsilon_p - \frac{3\pi N e^2}{4\epsilon R} \qquad l^2 := \frac{\hbar}{m^* \Omega}. \tag{15}$$

So all three quantities are now R-dependent, which should be kept in mind.

Note that for our case, i.e. for $N \gg 1$, one has $R \gg l$; so almost all single-particle wavefunctions should be exponentially small for $r \approx R$; therefore only a negligible number of electrons are located near the edge of the dot, and the solutions of equation (14) given by equations (3) and (4) can also be applied for $r > R$.

3.2. Thermodynamics

At $T > 0$ the probability of finding an electron of the dot in a state with an energy

$$\epsilon_p = \epsilon_{n_+, n_-, s_z} + \frac{3\pi N e^2}{4\epsilon R}$$

i.e. $E_p = \epsilon_{n_+, n_-, s_z}$, is defined by the Fermi distribution $n_s(\epsilon)$, i.e.

$$n_s(\epsilon_+ n_+ + \epsilon_- n_-) := \left[1 + \exp\left(\frac{\epsilon_+ n_+ + \epsilon_- n_- - \mu_s}{k_B T}\right)\right]^{-1} \tag{16}$$

where $\mu = \mu(T, N, B)$ is the chemical potential of the electrons in the dot, and, with $s = s_z = \pm\frac{1}{2}$,

$$\mu_{s_z} := \mu - \frac{\epsilon_+ + \epsilon_-}{2} - g^* \frac{\omega_c}{2} s_z - \frac{3\pi N e^2}{4\epsilon R} \qquad \epsilon_\pm := \hbar\Omega \pm \frac{1}{2}\hbar\omega_c. \tag{17}$$

The chemical potential μ can be determined as usual from the condition that $N = \sum_{s=-1/2}^{+1/2} N_s$, with

$$N_s(T, B, \mu) = \sum_{n_+=0}^{\infty} \sum_{n_-=0}^{\infty} n_s(\epsilon_+ n_+ + \epsilon_- n_-). \tag{18}$$

Let us now introduce the *grand thermodynamic potential* $\mathcal{Y}(T, B, \mu) = \sum_{s=-1/2}^{+1/2} \mathcal{Y}_s(T, B, \mu)$, through

$$\mathcal{Y}_s := \sum_{n_+, n_- = 0}^{\infty} \phi_s(\epsilon_+ n_+ + \epsilon_- n_-) \qquad \text{with } \phi_s(\epsilon) := -k_B T \ln \left[1 + \exp\left(\frac{\mu_s - \epsilon}{k_B T} \right)_{N, B} \right]. \quad (19)$$

Then the 'mean energy' $E(T, B, N)$ (i.e. the *internal enthalpy*[6] of the dot), and its *free enthalpy* $G(T, B, N) = E - TS$, where S is the entropy, are determined by the equations

$$E = \mathcal{Y} + \mu N - T \left(\frac{\partial \mathcal{Y}}{\partial T} \right) - \frac{9\pi}{20} \frac{N^2 e^2}{\epsilon R} \quad (20)$$

$$G = \mathcal{Y} + \mu N - \frac{9\pi}{20} \frac{N^2 e^2}{\epsilon R}. \quad (21)$$

Here the final term in equations (20) and (21) represents the 'double-counting correction' of the Coulomb energy, where we have used the fact that

$$\frac{e^2}{2\epsilon} \int d^2r \int d^2r' \frac{n(r)n(r')}{|\vec{r} - \vec{r}'|} = \frac{3\pi}{10} \frac{N^2 e^2}{\epsilon R}.$$

At $T \to 0$, E and G transform into the energy of the ground state of the dot:

$$E_0 = \lim_{T \to 0} E = \lim_{T \to 0} G = \mathcal{Y}_0 + \epsilon_F N - \frac{9\pi}{20} \frac{N^2 e^2}{\epsilon R_0}$$

where

$$\mathcal{Y}_0 := \lim_{T \to 0} \mathcal{Y} \qquad \epsilon_F := \lim_{T \to 0} \mu \qquad R_0 := \lim_{T \to 0} R.$$

Now for finite temperatures we define our 'effective dot radius' $R = R(N, B, T)$ (or more precisely: the 'effective radius of the electron liquid on the dot') from the condition that the free enthalpy should fulfil:

$$\left(\frac{\partial G}{\partial R} \right)_{|N, T, B} = 0. \quad (22)$$

Again, this condition couples spin and orbital degrees of freedom.

As in [10], we now use *Laplace transforms* of the quantities appearing in (18) and (19), marked by a 'tilde'; e.g. we write

$$n_s(\epsilon) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dp \, \tilde{n}_s(p) e^{+p\epsilon} \qquad \text{with } \tilde{n}_s(p) = \int_0^\infty d\epsilon \, n_s(\epsilon) e^{-p\epsilon}$$

where c is an arbitrary real number, which must only be 'positive enough' to ensure existence of the transformation (see below). Then N_s and $\mathcal{Y}_s$ can be represented in the following form:

$$N_s = \int_0^\infty \left(-\frac{\partial n_s(\epsilon)}{\partial \epsilon} \right) Z(\epsilon) \, d\epsilon \quad (23)$$

$$\mathcal{Y}_s = -\int_0^\infty n_s(\epsilon) Z(\epsilon) \, d\epsilon \quad (24)$$

---

[6] Since the Zeeman term '$-BM$' is included in the Hamiltonian $\mathcal{H}$, the expectation value $\langle \mathcal{H} \rangle$ is called the 'internal enthalpy' whereas the name 'internal energy' is reserved for the expectation value of those parts of $\mathcal{H}$, e.g. the 'exchange energy', which do depend on M, but not explicitly on B. In fact, the relation between the 'internal enthalpy' $I(T, B)$ and the 'internal energy' $U(T, M)$ is given by the *Legendre transform* $I(T, B) = U(T, M) - BM$.

where the Laplace transform of $Z(\epsilon)$ is given by the simple expression

$$\tilde{Z}(p) = \frac{1}{p(1 - e^{-\epsilon_+ p})(1 - e^{-\epsilon_- p})}. \tag{25}$$

Here the constant c in the Laplace transform (see above) has to be chosen in such a way that all singularities of $\tilde{Z}(p)$ are situated to the left of the straight line $(c - i\infty, c + i\infty)$—this gives a precise meaning to the above-mentioned formulation 'positive enough'; then the contour of integration in (25) can be closed at infinity, and we can use the calculus of residues to evaluate the integral. It is easy to show that $\tilde{Z}(p)$ has at the same time poles of first order at the points $p = p_n^{(\pm)} := 2\pi i n \hbar \Omega / \epsilon_{\pm}$, with $n = \pm 1, \pm 2, \ldots$, and a pole of third order at $p = 0$, if the quantity $X := \omega_c / (2\Omega)$ is $\neq X_0$, where

$$X_0 = 0, \frac{1}{3}, \frac{1}{5}, \frac{3}{5}, \ldots. \tag{26}$$

If, on the other hand, the non-generic condition $X = X_0$ is fulfilled, then $\tilde{Z}(p)$ has poles of first, second and third order.

From now on we will be interested only in the 'generic situation', i.e. in those fields for which $X \neq X_0$. Having found all the residues of $\tilde{Z}(p)$ and performing the summation with respect to all poles, we find an expression for $Z(\epsilon)$. Then, substituting $Z(\epsilon)$ into the integrals (23) and (24) and using the properties of the Fermi functions, we find expressions for N and $\mathcal{Y}$. In the low-temperature limit $k_B T \ll \mu_s$, these quantities take the form

$$N = \frac{\mu^2}{\epsilon_0^2} - \frac{1}{2} + ((g^*)^2 - 1)\left(\frac{\hbar\omega_c}{2\epsilon_0}\right)^2 + \frac{\pi^2}{3}\left(\frac{k_B T}{\epsilon_0}\right)^2$$

$$+ \sum_{s=-1/2}^{+1/2} \left\{ P_1^{(+)}\left(\frac{\mu_s\epsilon_+}{\epsilon_0^2}\right) - \frac{\epsilon_-}{\epsilon_+} P_2^{(+)}\left(\frac{\mu_s\epsilon_+}{\epsilon_0^2}\right)\right\}$$

$$+ \sum_{s=-1/2}^{+1/2} \left\{ P_1^{(-)}\left(\frac{\mu_s\epsilon_+}{\epsilon_0^2}\right) - \frac{\epsilon_+}{\epsilon_-} P_2^{(-)}\left(\frac{\mu_s\epsilon_-}{\epsilon_0^2}\right)\right\} \tag{27}$$

$$\mathcal{Y} = -\frac{1}{3}\frac{\mu^3}{\epsilon_0^2} + \frac{\mu}{2} - \mu((g^*)^2 - 1)\left(\frac{\hbar\omega_c}{2\epsilon_0}\right)^2 - \frac{\hbar\Omega}{2}\left[1 + \frac{4}{3}\left(\frac{\hbar\omega_c}{\epsilon_0}\right)^2\right]$$

$$- \mu\frac{\pi^2}{3}\left(\frac{k_B T}{\epsilon_0}\right)^2 + \epsilon_- \sum_{s=-1/2}^{+1/2} \left\{ P_1^{(+)}\left(\frac{\mu_s\epsilon_+}{\epsilon_0^2}\right) + \frac{\epsilon_-}{\epsilon_+} P_2^{(+)}\left(\frac{\mu_s\epsilon_+}{\epsilon_0^2}\right)\right\}$$

$$+ \epsilon_+ \sum_{s=-1/2}^{+1/2} \left\{ P_1^{(-)}\left(\frac{\mu_s\epsilon_+}{\epsilon_0^2}\right) + \frac{\epsilon_+}{\epsilon_-} P_2^{(-)}\left(\frac{\mu_s\epsilon_-}{\epsilon_0^2}\right)\right\} \tag{28}$$

where

$$\epsilon_0^2 := \hbar^2\left(\omega_0^2 - \frac{3\pi}{4}\frac{Ne^2}{\epsilon m^* R^3}\right)$$

which corresponds to the first equation in (15). Here the periodic functions $P_m^{(\pm)}(z)$ have for *even m* the form

$$P_m^{(\pm)}(z) = \sum_{n=1}^{\infty} \frac{2\pi^2 nkT\epsilon_{\pm}}{\epsilon_0^2}\left[\sinh\left(\frac{2\pi^2 nkT\epsilon_{\pm}}{\epsilon_0^2}\right)\right]^{-1}\frac{\cos(2\pi nz)}{2^{m-1}\pi^m n^m} \tag{29}$$

whereas for *odd m* the same result applies, if the functions $\cos(2\pi nz)$ in (29) are replaced by $\sin(2\pi nz)$.

Finally, we obtain the following expression for the free enthalpy:

$$G = \frac{2\mu^3}{3\epsilon_0^2} + \frac{9\pi N^2 e^2}{20\epsilon R} + \mu \sum_{s=-1/2} \left\{ P_1^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) + P_1^{(-)}\left(\frac{\mu_s \epsilon_-}{\epsilon_0^2}\right) \right\}$$

$$- \mu \sum_{s=-1/2} \left\{ \frac{\epsilon_-}{\epsilon_+} P_2^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) + \frac{\epsilon_-}{\epsilon_+} P_2^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) \right\}$$

$$+ \sum_{s=-1/2}^{+1/2} \left\{ \epsilon_- P_2^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) + \epsilon_+ P_2^{(-)}\left(\frac{\mu_s \epsilon_-}{\epsilon_0^2}\right) \right\}$$

$$+ \sum_{s=-1/2}^{+1/2} \left\{ \frac{\epsilon_-^2}{\epsilon_+} P_3^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) + \frac{\epsilon_+^2}{\epsilon_-} P_3^{(-)}\left(\frac{\mu_s \epsilon_-}{\epsilon_0^2}\right) \right\}$$

$$- \frac{\hbar\Omega}{2} \left[1 + \frac{4}{3}\left(\frac{\hbar\omega_c}{2\epsilon_0}\right)^2 \right]. \tag{30}$$

The chemical potential μ is found from (27), which can be rewritten as

$$\frac{\mu^2}{N\epsilon_0^2} = 1 + \frac{1}{N}\left\{ \frac{1}{2} - ((g^*)^2 - 1)\left(\frac{\hbar\omega_c}{2\epsilon_0}\right)^2 - \frac{\pi^2}{3}\left(\frac{k_B T}{\epsilon_0}\right)^2 \right\}$$

$$- \frac{1}{N}\left\{ \sum_{s=-1/2}^{1/2} \left[P_1^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) + P_1^{(-)}\left(\frac{\mu_s \epsilon_-}{\epsilon_0^2}\right) \right] \right\}$$

$$- \frac{1}{N}\left\{ \sum_{s=-1/2}^{1/2} \left[\frac{\epsilon_-}{\epsilon_+} P_2^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) + \frac{\epsilon_-}{\epsilon_+} P_2^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) \right] \right\}.$$

In the lowest approximation, if the number of electrons in the dot is large ($N \gg 1$), then at moderately low magnetic fields ($\hbar\omega_c \ll 2\epsilon_0$) and moderately low temperatures this expression takes the form (in the zeroth approximation, $\mu \approx \mu_0$) $\mu_0^2/(N\epsilon_0^2) = 1$, or $\mu \approx \mu_0 = \epsilon_0\sqrt{N}$.

In the next approximation, within an accuracy of order $1/\sqrt{N}$, the chemical potential is equal to

$$\mu \cong \epsilon_0\sqrt{N}\left\{ 1 + \frac{1}{2N} f(N, B, T) \right\} \tag{31}$$

where the quantity

$$f(N, B, T) = \frac{1}{2} - ((g^*)^2 - 1)\left(\frac{\hbar\omega_c}{2\epsilon_0}\right)^2 - \frac{\pi^2}{3}\left(\frac{k_B T}{\epsilon_0}\right)^2$$

$$- \sum_{s=-1/2}^{1/2} \left[P_1^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) + P_1^{(-)}\left(\frac{\mu_s \epsilon_-}{\epsilon_0^2}\right) \right]$$

$$- \sum_{s=-1/2}^{1/2} \left[\frac{\epsilon_-}{\epsilon_+} P_2^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) + \frac{\epsilon_-}{\epsilon_+} P_2^{(+)}\left(\frac{\mu_s \epsilon_+}{\epsilon_0^2}\right) \right]$$

is $\mathcal{O}(1)$, and from (17) one gets

$$\mu_s \approx (\mu_0)_{s_z} = \epsilon_0\sqrt{N} + \sqrt{\epsilon_0^2 + \left(\frac{\hbar\omega_c}{2}\right)^2} - g^* \frac{\hbar\omega_c}{2} s_z - \frac{3\pi N e^2}{4\epsilon R}.$$

If we substitute this expression for $\mu(N, B, T)$ in (30), we obtain the free enthalpy as a function of N, B, and T. As follows from (31), the first summand in the r.h.s. of (30) is of order $N^{3/2-2\sigma}$,

if $\epsilon_0 \sim N^\sigma$ (it can be shown that $\sigma = 1/6$; see equation (33) below). The second summand on the r.h.s. of (30) is of order $N^{2-\gamma}$ (with $\gamma = \frac{1}{3}$; see (33)). All other summands have still less order of magnitude. If we retain only the first two terms in the r.h.s. of (30) and use (22), then we come to the following equation for R [10]:

$$\omega_0^2 \cong \left(\frac{3\pi}{4} \frac{Ne^2}{\epsilon R^3 m^*} \right) \left\{ 1 + \frac{100 a_B^*}{27\pi R} \right\} \tag{32}$$

where $a_B^* := \hbar^2 \epsilon / (m^* e^2)$ is the *effective Bohr radius*.

This means that ω_0 ($=\epsilon_0/\hbar$) is essentially identified with the plasma frequency calculated from the electron density in the dot calculated with $T = 0$ and $B = 0$; in this approximation the radius R of the dot does not depend on B and T at all and is defined only by the number N of electrons on the dot. To obtain a dependence of R on B and T while solving equation (32), it is in principle necessary to take into account corrections of higher order; yet at $N \gg 1$ the corrections are very small, namely relatively $\mathcal{O}(N^{-1/2})$, and we neglect them.

For $a_B^* \ll R$ the solution of (32) in the first approximation is

$$R \cong R_0 \left(1 + \frac{100 a_B^*}{51\pi R_0} \right) \tag{33}$$

where

$$R_0 := \left(\frac{3\pi Ne^2}{4\epsilon m^* \omega_0^2} \right)^{1/3}.$$

Hence

$$\epsilon_0 = \hbar \left[\omega_0^2 - \frac{3\pi Ne^2}{4\epsilon m^* R^3} \right]^{1/2} = \hbar \omega_0 \left[\left(\frac{100 a_B^*}{27\pi R} \right) \middle/ \left(1 + \left(\frac{100 a_B^*}{27\pi R} \right) \right) \right]^{1/2} \propto R^{-1/2} \propto N^{-1/6}$$

and

$$\frac{9\pi^2 N^2 e^2}{20\epsilon R} \propto \frac{N^2}{R} \propto N^{2-1/3}$$

as already stated above.

From equation (32) it follows that R transforms into R_0 in the classical limit ($\hbar \to 0$); cf. equation (12). Moreover, the dependence of R with respect to N and $\hbar\omega_0$ as above corresponds well to numerical results from [8].

Now the magnetic moment of a dot is defined by the derivative

$$M = -\left(\frac{\partial \mathcal{Y}}{\partial B} \right)_{\mu, T}.$$

Using expression (29) for $\mathcal{Y}$ we find M, taking into account terms of order $1/\sqrt{N}$:

$$\frac{M}{\mu_B^*} = \sqrt{N} \left[((g^*)^2 - 1) \frac{\mu_B^* B}{\epsilon_0} + 2 \frac{P_1^{(+)}(\mu_0 \epsilon_+/\epsilon_0^2) - P_1^{(-)}(\mu_0 \epsilon_-/\epsilon_0^2)}{\sqrt{1 + (\mu_B^*)^2 B^2 / \epsilon_0^2}} \right] \tag{34}$$

where $\mu_0 = \epsilon_0 \sqrt{N}$ has been defined above.

We see from this expression that $M \to 0$ for $B \to 0$, since then $\epsilon_+ = \epsilon_-$. At the same time the first summand on the r.h.s. of (34) is *negative* ($(g^*)^2 < 1$) and *monotonically decreasing* with increasing B. However, the second summand *oscillates* around zero with increasing B, and so the possibility exists that $(1/B)M/\mu_B^*$ may be *positive* at $B \to 0$. Let us find the conditions in which this case can happen.

To do this we expand the r.h.s. of (34) into a series in terms of B, and in a linear approximation in B we get for $N \gg 1$

$$\frac{M}{\mu_B^*} = \sqrt{N}((g^*)^2 - 1)\frac{\mu_B^* B}{\epsilon_0} + 4N P_0(\sqrt{N})\frac{\mu_B^* B}{\epsilon_0} \approx 4N P_0(\sqrt{N})\frac{\mu_B^* B}{\epsilon_0}. \quad (35)$$

The function $P_0(x)$ is periodic, with period $\Delta x = 1$, i.e.

$$P_0(x) = 2\sum_{n=1}^{\infty} \frac{2\pi^2 n k_B T}{\epsilon_0}\left[\sinh\left(\frac{2\pi^2 n k_B T}{\epsilon_0}\right)\right]^{-1}\cos(2\pi n x) \quad (36)$$

which can also be written as

$$P_0(x) = \left\{\sum_{n=-\infty}^{+\infty} A(x - n)\right\} - 1$$

where the functions $A(x - n)$ are calculated in the appendix. As a consequence of the large-n behaviour of the Fourier coefficients in front of $\cos(2\pi n x)$ in (36), the function $A(x)$ reaches a sharp maximum at $x = 0$; that is,

$$A(x) \equiv \frac{\epsilon_0}{4k_B T}\left[\cosh\left(\frac{\epsilon_0 x}{2k_B T}\right)\right]^{-2} \to A(0) = \frac{\epsilon_0}{4k_B T}.$$

Thus the function $P_0(\sqrt{N})$ in equation (35) takes positive values at $N = m^2$ ($m = 0, 1, 2, \ldots$), if at the same time $\epsilon_0/(4k_B T) > 1$ (see also equation (37) below).

Therefore at low fields the quantity $M/(B\mu_B^*)$ is positive, if the following two conditions are simultaneously fulfilled: (i) the temperature has to be low enough: $T < T_0 := \epsilon_0/(4k_B)$; and (ii) the number N of electrons in the dot is equal to $N = m^2$, with $m = 0, 1, 2, \ldots$ (which corresponds for $B = 0$ to a 'half-filled-outer-shell' condition, as we shall see).

In fact, for a planar parabolic dot in the absence of magnetic field B and in a one-electron approximation without interaction, the energy levels of the electron are defined by quantum numbers $n = 0, 1, 2, \ldots$ ($=n_+ + n_-$ in equation (4)) and are degenerate with respect to the numbers

$$n_+ - n_- = \begin{cases} 0; \pm 2; \pm 4; \ldots; \pm n & \text{for even } n \\ \pm 1; \pm 3; \pm 5; \ldots; \pm n & \text{for odd } n \end{cases}$$

and, of course, also degenerate with respect to the spin.

Electronic states of a planar dot with the same quantum number n form a 'shell': then at $N = m^2$ the last electron shell (i.e. with the highest possible n) of the parabolic dot turns out to be just half-filled.

(Here it should be noted that in equation (35) the explicit spin dependence—i.e. the term involving $(g^*)^2$—is negligible for $N \gg 1$, and the phenomenon considered is actually primarily a shell effect.)

As a consequence, a planar quantum dot with $N = m^2$ ($\gg 1$), at low temperatures (namely $T < T_0 = \epsilon_0/(4k_B)$) and at 'sufficiently low fields' (what this means quantitatively is determined shortly), i.e. for $B \to 0$, turns out to be a 'paramagnetic two-dimensional artificial atom' with magnetic moment

$$M(T, B, N) = \mu_B^* 4N\left(\frac{\epsilon_0}{4k_B T} - 1\right)\frac{\mu_B^* B}{\epsilon_0}. \quad (37)$$

Thus, when the magnetic field is increased, the magnetic moment of a planar dot in a two-dimensional electron gas at first increases $\propto B$ according to (37); then, according to (34) it reaches a maximum, then diminishes again, vanishes, and becomes negative.

Let us first find the value B_0 where M vanishes. At $N = m^2$, i.e. at integer $\sqrt{N}$, we have

$$P_1^{(\pm)}\left(\frac{\mu_0\epsilon_\pm}{\epsilon_0^2}\right) \approx P_1\left\{\sqrt{N}\left(1 \pm \frac{\mu_B^* B}{\epsilon_0}\right)\right\} \equiv \pm P_1\left(\sqrt{N}\frac{\mu_B^* B}{\epsilon_0}\right)$$

where $P_1(x)$ has been defined above. Then

$$\frac{M}{\mu_B^*} = \sqrt{N}\left\{((g^*)^2 - 1)\frac{\mu_B^* B}{\epsilon_0} + 4P_1\left(\sqrt{N}\frac{\mu_B^* B}{\epsilon_0}\right)\right\}. \tag{38}$$

If $T \to 0$, then at $0 < x < 1$ we have $P_1(x) \cong \frac{1}{2} - x$. That is why at $T = 0$ for sufficiently small magnetic fields

$$\frac{M}{\mu_B^*} = \sqrt{N}\left\{((g^*)^2 - 1)\frac{\mu_B^* B}{\epsilon_0} + 2 - 4\sqrt{N}\frac{\mu_B^* B}{\epsilon_0}\right\}.$$

The r.h.s. of this expression is positive when

$$B < B_0 := \frac{2\epsilon_0}{(4\sqrt{N} + 1 - (g^*)^2)\mu_B^*} \approx \frac{\epsilon_0}{2\sqrt{N}\mu_B^*}. \tag{39}$$

So 'sufficiently small fields' means $B \ll B_0$; i.e. in the region $(B < B_0, T < T_0)$ the magnetic moment of a planar dot is positive (i.e. the dot is *paramagnetic*). Outside this region M is $\leqslant 0$, and the dot is *diamagnetic*.

For GaAs at $\hbar\omega_0 = 3.37$ meV we have the following typical values for T_0 and B_0, which should be compared with the results of figures 2, 3:

$$N = 100 \qquad T_0 = 3.26 \text{ K} \qquad B_0 = 0.065 \text{ T}$$
$$N = 25 \qquad T_0 = 4.10 \text{ K} \qquad B_0 = 0.164 \text{ T}.$$

As in the case of a dot with $N = 1$ electron, finally the *adiabatic temperature derivative* $(\mathrm{d}T/\mathrm{d}B)_S$ w.r.t. changes of the magnetic field is calculated through the expression

$$\left(\frac{\mathrm{d}T}{\mathrm{d}B}\right)_S = -T\frac{(\partial M/\partial T)_{B,N}}{C_{B,N}}$$

where $C_{B,N}$ is the heat capacity of the dot. From (27) and (28) it is easy to show that

$$C_{B,N} = \sqrt{N}\frac{2\pi^2}{3}\frac{k_B^2}{\epsilon_0} + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right).$$

If we consider dots with half-filled last electron shells (i.e. $N = m^2$), then according to (38)

$$\left(\frac{\partial M}{\partial T}\right)_{B,N} = 4\mu_B^* \frac{\partial}{\partial T}P_1\left(\sqrt{N}\frac{\mu_B^* B}{\epsilon_0}\right).$$

(Here one should remember that $P_1(x)$ depends on T; see equation (29).)

Hence it follows that

$$\left(\frac{\mathrm{d}T}{\mathrm{d}B}\right)_S = -4\mu_B^*\left(\sqrt{N}\frac{2\pi^2}{3}\frac{k_B^2}{\epsilon_0}\right)^{-1}\frac{\partial}{\partial T}P_1\left(\sqrt{N}\frac{\mu_B^* B}{\epsilon_0}\right). \tag{40}$$

If we use the relationship

$$\frac{\partial P_1(x)}{\partial x} = P_0(x)$$

and the expression (36) for $P_0(x)$, then it is possible to show that at $0 < x < 1$

$$P_1(x) = \frac{1}{2}\sum_{n=-\infty}^{+\infty}\tanh\left[\frac{\epsilon_0(x - n)}{2k_B T}\right] - x + \frac{1}{2}.$$

Hence it follows that the derivative $\partial P(x)/\partial T$ vanishes at $x = 0, \frac{1}{2}, 1$. At the same time

$$\frac{\partial^2 P_1(x)}{\partial x\,\partial T}\bigg|_{x=0} = \frac{\partial^2 P_1(x)}{\partial x\,\partial T}\bigg|_{x=1} = -\frac{\epsilon_0}{4k_B T^2} < 0$$

whereas

$$\frac{\partial^2 P_1(x)}{\partial x\,\partial T}\bigg|_{x=1/2} > 0.$$

Thus, at low fields ($\sqrt{N}\mu_B^* B/\epsilon_0 \ll 1$), like for $N = 1$ (see figure 2), we get *positive* values of the adiabatic temperature derivative:

$$\left(\frac{\mathrm{d}T}{\mathrm{d}B}\right)_S = \frac{3}{2\pi^2}\frac{\epsilon_0(\mu_B^*)^2}{k_B(k_B T)^2}B > 0. \tag{41}$$

Altogether this means that the temperature obtained by adiabatic demagnetization of the dots, $\mathrm{d}B < 0$, is strongly B-dependent: it *first diminishes with decreasing B*, then reaches a minimum value at $B = B_k := \epsilon_0/(2\sqrt{N}\mu_B^*)$ (since the derivative $(\mathrm{d}T/\mathrm{d}B)_S$ vanishes at $\sqrt{N}\mu_B^* B/\epsilon_0 = \frac{1}{2}$, i.e. $B = B_k$), and then begins to *rise*, due to the fact that $(\mathrm{d}T/\mathrm{d}B)_S < 0$ at $B > B_k$.

As regards the B-dependence of $(\mathrm{d}T/\mathrm{d}B)_S$, we mention—however—the following point: for $N = 1$, the contour line $(\mathrm{d}T/\mathrm{d}B)_S = 0$ in figure 2 depends on T only, but not on B, for a large region of B-values, where it is simply given by $T \approx 3$ K. According to figure 2, this seems only to be different for very small B-values at $T > 3$ K. In the former respect there seems to be a qualitative distinction between the cases $N = 1$ and $N \gg 1$, which we do not understand at present.

Finally, using expression (41), let us find out *how fast* the temperature of a dot is diminished or increased by the adiabatic change of the magnetic field: if we let in (41) $T_S(B) = T + \Delta T(B)$, where T is the initial temperature, $T_S(B)$ the final temperature, and $\Delta T(B) \ll T$, then it is easy to show that

$$\Delta T(B) \approx \frac{3}{4\pi^2}\left(\frac{\epsilon_0}{k_B T}\right)^3\left(\frac{\mu_B^* B}{\epsilon_0}\right)^2 T. \tag{42}$$

Thus for quantum dots in a two-dimensional electron gas with GaAs parameters at a start temperature of e.g. $T = 2$ K, and with a 'confining energy' $\epsilon_0 = \hbar\omega_0 = 3.37$ meV, if one wants to change the electron temperature on the dot by $\Delta T = \pm 0.1$ K for $N = 100$, the B-field only needs to change by ± 0.063 T; and for $N = 25$, it only needs to change by ± 0.057 T. If $\hbar\omega_0 = 7.5$ meV, then at $N = 100$ the field has to change by ± 0.04 T and at $N = 25$ by ± 0.035 T.

Finally the following points should be mentioned: as a consequence (i) of a pronounced B-dependence of the total-angular-momentum quantum numbers $L(B)$ and $S(B)$ of the ground state of the electronic ensemble and (ii) of the Coulomb interaction of the electrons, oscillations of the physical properties of quantum dots with B have already been predicted and observed in a number of papers; e.g. even in an early paper of Dingle [16], before the invention of quantum dots, and later on in papers of Maksym and Chakraborty [7], and in [12]. Furthermore, numerical results for *small* numbers of electrons, $N = \mathcal{O}(10)$, show that the maximum electron density may not be at the origin for all electron numbers and magnetic fields (see e.g. [8, 9, 14, 17]), and that the 'electronic edge' of the quantum dot may get a non-trivial structure, i.e. the 'edge reconstruction' [2, 9]. However, here we stress for $N \gg 1$ that

(i) in principle the orbital and spin degrees of freedom are intrinsically coupled for the individual electrons, although of course the total momentum quantum numbers S and L remain well defined for circular dots; and that

(ii) with the quasi-classical electron density (12) it follows from equation (39) that there are not only periodic oscillations of the magnetization of the dots with a period $\propto B\sqrt{N}/\epsilon_0$, but that throughout these oscillations, M does not remain negative but alternates periodically in sign. This is essentially a 'Hartree shell effect', and it seems from our analytical results that this should be seen parallel to the exchange mechanisms, i.e. one is dealing—as one might say—with two different sides of one coin. This is analogous to the situation in the conventional 3d magnetism, where both the 'Hubbard mechanism' (in mean-field approximation essentially a Hartree effect) and the 'Hund's-rule exchange' are important for the magnetic properties, although of different relative importance for different systems.

4. Conclusions

It follows from the above statements that:

- The magnetization of a planar one-electron dot, $N = 1$, see (6), can be separated into two parts: (i) the *paramagnetic* magnetization caused by the magnetic *spin momentum* of the electron itself; and (ii) the orbital magnetization which is due to the quantized *orbital* motion of the electron of the dot in a magnetic field. At low temperatures ($T < T_0$) and fields ($B < B_0$) the paramagnetic part of the susceptibility exceeds the diamagnetic one, and as a whole the dot is paramagnetic, whereas at high fields and temperatures, the dot behaves diamagnetically. An analogous situation is observed concerning the *adiabatic temperature derivative* w.r.t. changes of the magnetic field: at low fields ($B < B_k$) and temperatures ($T < T_k$), the adiabatic temperature derivative $(\mathrm{d}T/\mathrm{d}B)_S$ is >0, whereas it is <0 at high fields and temperatures. For more results for GaAs parameters, figure 2 and figure 3 should be consulted, and it should be noted that in the case of figure 3 one obtains quite pronounced effects in the 'sensitive region' of $T \approx 1.5$ K for $B \lesssim 0.002$ T.

- In a many-electron planar dot ($N \gg 1$), the effects of quantization of orbital motion and the spin effects cannot be separated and should be treated simultaneously. We do this within a simplified Hartree approach leading to a renormalized single-particle equation, where the effective radius R of the electron liquid on the dot is used as fitting parameter to minimize the free enthalpy of the system at finite temperatures. In this way, orbital and spin degrees of freedom are now coupled in a rather subtle way.

  With increasing B, for $N \gg 1$, a spin-dependent restructuring of energy levels takes place. As a consequence of a shell effect, this leads to a *periodic* change of the magnetic properties of the electrons in a dot with varying B, which is a function of the variable

$$x := \frac{\sqrt{N}\hbar|e|B}{2m^*c\epsilon_0}$$

  with period $\Delta x = 1$. (Here all parameters have their usual meaning, and $\epsilon_0 = \hbar\omega_0$ is the confinement energy. It should be noted that the period does not depend on the temperature and involves only the characteristic energy scales of the system, except for the factor $\sqrt{N}$. The factor $\sqrt{N}$ itself is of course related to the above-mentioned condition of a half-filled outer shell, $N = m^2$.) Furthermore, the magnetic susceptibility of a dot with a half-filled last electron shell changes not only in magnitude, but also in sign: for low fields ($B < B_0$) and temperatures ($T < T_0$), the dot as a whole is paramagnetic, whereas with increasing B and T, the behaviour of the dot transforms from paramagnetic to diamagnetic.

  In an analogous manner, the temperature effect induced by adiabatic demagnetization of the dot behaves differently at low temperatures and fields ($T < T_k$, $B < B_k$) and at high fields ($B > B_k$), respectively: in the former case, the temperature diminishes with adiabatic decrease of B, whereas in the second case, it rises.

Acknowledgments

Appendix

In this appendix we derive the relation between the periodic function $P_0(x)$, given by the 'Bloch representation' equation (36), and the corresponding 'Wannier representation', given by the functions $A(x-n)$.

The periodic function $P_0(x) \, (=P_1'(x))$ is

$$P_0(x) = 2 \sum_{n=1}^{\infty} \tilde{A}(n) \cos(2\pi nx) = \left\{ \sum_{n=-\infty}^{+\infty} \tilde{A}(n) e^{i 2\pi nx} \right\} - 1$$

where

$$\tilde{A}(n) = \frac{2\pi^2 n k_B T}{\epsilon_0} \left[\sinh\left(\frac{2\pi^2 nkBT}{\epsilon_0} \right) \right]^{-1}.$$

Using the identity

$$\sum_{n=-\infty}^{+\infty} \delta(x-n) = \sum_{n=-\infty}^{+\infty} \exp(-i 2\pi nx)$$

we find

$$P_0(x) = \left\{ \int_{-\infty}^{+\infty} \tilde{A}(k) e^{2\pi i(x-n)} \, dk \sum_{n=-\infty}^{+\infty} \delta(k-n) \right\} - 1$$

$$= \int_{-\infty}^{+\infty} \tilde{A}(k) \, dk \sum_{n=-\infty}^{+\infty} e^{2\pi i(x-n)} - 1 = \sum_{n=-\infty}^{+\infty} A(x-n) - 1$$

with

$$A(x) = \int_{-\infty}^{+\infty} \tilde{A}(k) e^{2\pi ikx} \, dk \equiv \frac{\epsilon_0}{4k_B T} \left[\cosh\left(\frac{\epsilon_0 x}{2k_B T} \right) \right]^{-2}.$$

References

[1] This point of view is e.g. stressed in a recent preprint of Loss *et al*:
   Recher P, Loss D and Levy J 2000 Spintronics and quantum computing with quantum dots *Preprint* cond-mat/0009270
[2] Jacak L, Hawrylak P and Wójs A 1997 *Quantum Dots* (Berlin: Springer)
[3] Vonsovskij S V 1971 *Magnetism* (Moscow: Nauka) (in Russian)
[4] Back C H, Allenspach R, Weber W, Parkin S S P, Weller D, Garwin E L and Siegmann H C 1999 *Science* **285** 864
[5] Leineweber T and Kronmüller H 1999 *J. Magn. Magn. Mater.* **192** 575
[6] Awschalom D D and Kikkawa J M 1999 *Phys. Today* **52** (6) 33
[7] Maksym P A and Chakraborty T 1992 *Phys. Rev.* B **45** 1947
[8] Maksym P A 1996 *Phys. Rev.* B **53** 10871
[9] Chamon C de C and Wen X G 1994 *Phys. Rev.* B **49** 8227
[10] Jacak L, Krasnyj Yu and Wójs A 1997 *Physica* B **229** 279
[11] Landau L D and Lifshitz E M 1977 *Quantum Mechanics; Non-Relativistic Theory (Course of Theoretical Physics vol 3)* (Oxford: Pergamon)
[12] Wagner M, Merkt U and Chaplik A 1992 *Phys. Rev.* B **45** 1951

[13] Shikin V, Nazin S, Heitmann D and Demel T 1991 *Phys. Rev.* B **43** 11 903

[14] Pfannkuche D, Gudmundson V and Maksym P A 1993 *Phys. Rev.* B **47** 2244

[15] Vignale G and Rasolt M 1988 *Phys. Rev.* B **37** 10 685

[16] Dingle R B 1952 *Proc. R. Soc.* A **211** 500

[17] Reimann S M, Koskinen M, Manninen M and Mottelson B R 1999 *Phys. Rev. Lett.* **83** 3270