

Spin–orbit interaction in the quantum dot

Lucjan Jacak^{a,*}, Jurij Krasnyj^b, Arkadiusz Wójs^a

^a*Institute of Physics, Technical University of Wrocław, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland*

^b*Institute of Physics, University of Odessa, Petra Velikogo 2, Odessa 270100, Ukraine*

Received 20 June 1996

Abstract

The electronic states of a parabolic quantum dot in a magnetic field are studied with the inclusion of the spin–orbit interaction. The analytical formulae for the ground state energy of the interacting system are derived. The spin–orbit interaction is shown to introduce new features to the far infrared absorption spectrum, where it leads to the splitting of the two principal modes. The results are compared with the charging experiments by Ashoori et al. and the far infrared absorption measurements by Demel et al.

Keywords: Spin–orbit interaction; Quantum dot; Electronic state

1. Introduction

Recent progress in the semiconductor nanostructure technology has allowed for creation of the quasi-zero-dimensional (0D) systems known as quantum dots [1]. These structures can be obtained e.g. by applying spatially modulated electric field to the 2D electron gas [2,3], or by embedding a small piece of one semiconductor into another, with higher conduction band energy (this can be achieved e.g. through etching [4–7], interdiffusion [8] or self-organized growth [9,10]). The resulting lateral potential is often very well approximated by the isotropic parabola [11–13]. The confinement in all three spatial directions leads to a discrete energy spectrum of the system with characteristic excitation energies of the order of few meV, which can be studied using the spectroscopy methods [2–5].

Due to the so-called generalized Kohn theorem [14,15] for the parabolic confinement the electron–electron Coulomb interaction does not affect the resonance energy spectrum under the far infrared (FIR) radiation. The FIR resonant spectrum of the corre-

lated many-electron dot is therefore identical to that of a single electron and consists of two degenerate modes. The degeneracy can be removed by a perpendicular magnetic field under which the two modes evolve into the inter-Landau-level (cyclotron) and intra-Landau-level frequencies. However, a number of experiments seem to show a slight dependence of the two resonance energies on the number of electrons in the dot [3–5]. Moreover, a small splitting of the two principal modes is observed [4] what reveals their additional sub-level structure.

The theoretical investigations of the ground state of quantum dots containing 2–15 electrons were reported e.g. in Refs. [15–20]. In this paper we calculate analytically the ground state energy of a system of a larger number of confined electrons ($\sim 15 - 100$) within a Hartree–Fock approximation. The spin–orbit interaction is included here in the manner analogous to that used for many-electron atoms and not via the *bulk* band-structure parameters, since the considered system is strongly localized (diameter ~ 20 lattice constants [4]) and the small piece of crystal, to which the motion of electrons is limited, cannot be treated as an infinite periodical lattice. Instead, we propose to

* Corresponding author.

extract the spin–orbit coupling from the band-structure description and include it later on the level of the Bloch envelope wave functions by adding the appropriate term to the Hamiltonian. As demonstrated by Darnhofer and Rössler [19] for two electrons, inclusion of the spin–orbit interaction through the band-structure parameters in the InSb dot leads to the similar effects on the electronic structure as obtained here for the GaAs dots (spin–orbit coupling in bulk InSb significantly exceeds that in bulk GaAs).

The results obtained within proposed here framework seem to explain a number of experimentally observed effects, like an appearance of the higher modes in FIR absorption and their anti-crossing in a magnetic field [4] or the characteristic bumps in the magnetic field dependence of the ground state energy [6]. Let us also underline that we managed to fit very well the characteristic magnetic field at which the anti-crossing in FIR spectrum and the bumps in energy occur. The fact that this was impossible without including the spin–orbit interaction (see the numerical results and discussion by Palacios et al. [20] for up to 15 electrons) seems to prove the importance of this effect.

2. Model

The interaction between the spin and orbital angular momentum: σ and l , of an electron confined in a quasi-two-dimensional quantum dot is included in the way analogous to that used in many-electron atoms, i.e. via the single-particle potential:

$$V_{LS} = \alpha \mathbf{l} \cdot \boldsymbol{\sigma}. \quad (1)$$

The coupling constant α is connected with the average self-consistent field $\langle \delta U \rangle$ acting on the electron, via the relation

$$\alpha = \beta \langle \delta U \rangle. \quad (2)$$

For a Z -electron atom the dimensionless parameter β is

$$\beta = \left(\frac{Ze^2}{\hbar c} \right)^2 \approx \left(\frac{Z}{137} \right)^2. \quad (3)$$

In the case of a quantum dot β will be treated as a fitting parameter, while the magnitude of the field

$\langle \delta U \rangle$ will be estimated according to the electronic structure of the dot.

Let us write the total Hamiltonian of a system of many electrons, in the effective mass approximation, including the kinetic energy in the perpendicular magnetic field B , parabolic confinement of the characteristic frequency ω_0 , spin–orbit coupling as above, the Zeeman splitting for the effective g -factor and the electron–electron Coulomb interaction controlled by the dielectric constant ε :

$$\begin{aligned} \mathcal{H} &= \sum_i \left[\frac{1}{2m^*} \left(\mathbf{p}_i + \frac{e}{c} \mathbf{A}_i \right)^2 + \frac{1}{2} m^* \omega_0^2 r_i^2 \right. \\ &\quad \left. + \alpha l_i \sigma_i - g \mu_B \sigma_i B \right] + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{\varepsilon |\mathbf{r}_i - \mathbf{r}_j|} \\ &\equiv \sum_i (H_B)_i + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{\varepsilon |\mathbf{r}_i - \mathbf{r}_j|}. \end{aligned} \quad (4)$$

In the above m^* is the effective mass, \mathbf{r} are the positions, $\mathbf{p} = -i\hbar \nabla$ are the momenta, $\mathbf{A} = \frac{1}{2} B(y, -x, 0)$ are the vector potentials in the symmetric gauge, l and σ are the projections of the orbital angular momentum l and spin σ across the plane of motion.

In the Hartree–Fock (HF) approximation the equation for the HF wave functions ψ reads

$$\begin{aligned} [H_B + V_i] \psi_i(\mathbf{r}\sigma) + \sum_{\sigma'} \int d\mathbf{r}' \Delta_i(\mathbf{r}\sigma, \mathbf{r}'\sigma') \psi_i(\mathbf{r}'\sigma') \\ = \varepsilon_i \psi_i(\mathbf{r}\sigma), \end{aligned} \quad (5)$$

where H_B is the Hamiltonian of a single (non-interacting) electron for the field B defined in Eq. (4), V_i denotes the Hartree potential

$$V_i = \frac{e^2}{\varepsilon} \int d\mathbf{r}' \frac{n_i(\mathbf{r}')}{|\mathbf{r}' - \mathbf{r}|}, \quad (6)$$

with

$$n_i(\mathbf{r}) = \sum_{\sigma} \sum_j' |\psi_j(\mathbf{r}\sigma)|^2, \quad (7)$$

and Δ_i is the Fock correction:

$$\Delta_i(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -\frac{e^2}{\varepsilon} \delta_{\sigma'\sigma} \sum_j' \frac{\psi_j^*(\mathbf{r}'\sigma') \psi_j(\mathbf{r}\sigma)}{|\mathbf{r}' - \mathbf{r}|}. \quad (8)$$

Introducing the exchange operator G as

$$G_i \psi_i(\mathbf{r}\sigma) = \sum_{\sigma'} \int d\mathbf{r}' \Delta_i(\mathbf{r}\sigma, \mathbf{r}'\sigma') \psi_i(\mathbf{r}'\sigma'), \quad (9)$$

the HF equations (Eq. (5)) can be written in a compact form:

$$[H_B + V_i + G_i] \psi_i(\mathbf{r}\sigma) = \varepsilon_i \psi_i(\mathbf{r}\sigma). \quad (10)$$

Following the work by Shikin et al. [21] we employ here the approximate formula for the charge density in the parabolic dot (of confining frequency ω_0), obtained within the classical regime and therefore applicable for large numbers of electrons N :

$$n(r) = \begin{cases} n(0) \frac{1}{R} \sqrt{R^2 - r^2} & \text{for } r \leq R, \\ 0 & \text{for } r > R, \end{cases} \quad (11)$$

with the charge density in the center $n(0) = 3N/2\pi R^2$. The dot radius R , for the classical system given explicitly in Ref. [21] will be calculated here in a variational manner (from the minimum energy condition) in order to account for the quantum corrections. Using the formula (11) the Hartree potential is calculated:

$$V_R(r) = \frac{3\pi N e^2}{4\epsilon R} \left(1 - \frac{r^2}{2R^2} \right) \quad (12)$$

(we take this form also for $r > R$).

3. Quantum dot at zero magnetic field

3.1. Single-electron states

Let us first consider the case of zero magnetic field. Neglecting for the moment the exchange term (which will be included later as a perturbation) we obtain the following Hartree equations:

$$\begin{aligned} & \left(-\frac{\hbar^2}{2m^*} \Delta + \frac{1}{2} m^* \Omega_0^2 r^2 + \alpha l \sigma \right) \psi_i(\mathbf{r}\sigma) \\ & = \left(\varepsilon_i - \frac{3\pi N e^2}{4\epsilon R} \right) \psi_i(\mathbf{r}\sigma), \end{aligned} \quad (13)$$

where we use the effective frequency, renormalized by the Hartree term (Eq. (12)):

$$\Omega_0'^2 = \omega_0^2 - \frac{3\pi N e^2}{4\epsilon m^* R^3}. \quad (14)$$

Eq. (13) can be solved analytically and the obtained eigenstates are

$$\psi_i(\mathbf{r}\sigma) = \psi_{nm\sigma}(\mathbf{r}\sigma) = \phi_m(\theta) R_{nm}(r) \chi_\sigma, \quad (15)$$

with the spin eigenfunction χ_σ (with eigenvalues $\sigma = \pm \frac{1}{2} \hbar$), the angular wave function of the angular momentum eigenvalue m

$$\phi_m(\theta) = \frac{1}{\sqrt{2\pi}} e^{im\theta} \quad (16)$$

and the orbital wave function

$$\begin{aligned} R_{nm}(r) &= \frac{\sqrt{2}}{l_0'} \sqrt{\frac{n_r!}{(n_r + |m|)!}} \left(\frac{r}{l_0'} \right)^{|m|} \\ &\times e^{-r^2/2l_0'^2} L_{n_r}^{|m|} \left(\frac{r^2}{l_0'^2} \right). \end{aligned} \quad (17)$$

In the above $L_{n_r}^{|m|}$ are the Laguerre polynomials:

$$L_{n_r}^{|m|}(z) = \frac{1}{m!} z^{-|m|} e^z \frac{d^{n_r}}{dz^{n_r}} (z^{n_r + |m|} e^{-z}), \quad (18)$$

$l_0' = \sqrt{\hbar/m\Omega_0'}$ is the characteristic length, $n = 0, 1, 2, \dots$ is the principal quantum number, m is the azimuthal quantum number ($|m| \leq n$ and the parity of m is the same as that of n), and $n_r = \frac{1}{2}(n - |m|)$ is the radial quantum number.

The eigenenergies associated with the eigenfunctions $\psi_{nm\sigma}$ are

$$\varepsilon_{nm\sigma} = \hbar \Omega_0'(n + 1) + \alpha m \sigma + \frac{3\pi N e^2}{4\epsilon R}. \quad (19)$$

In the absence of the spin-orbit interaction ($\alpha = 0$) they form degenerate shells labelled by n . Non-vanishing α splits these shells into the doubly degenerate sub-levels.

Often used is a complementary (Fock–Darwin) representation

$$\psi_i(\mathbf{r}\sigma) = \psi_{n_+, n_-, \sigma}(\mathbf{r}\sigma) = \phi_{n_+, n_-}(\mathbf{r}) \chi_\sigma, \quad (20)$$

with $n_\pm = 0, 1, 2, \dots$. The two sets of quantum numbers: $[n, m]$ and $[n_+, n_-]$ are connected by the simple relations: $n = n_+ + n_-$ and $m = n_+ - n_-$. The orbital part of ψ_i is defined as

$$\psi_{n_+, n_-}(\mathbf{r}) = \frac{1}{\sqrt{2\pi} l_0'} \frac{(a^+)^{n_+} (b^+)^{n_-}}{\sqrt{n_+! n_-!}} e^{-r^2/2l_0'^2}, \quad (21)$$

where the raising operators a^+ and b^+ are

$$\begin{aligned} a^+ &= \frac{1}{2i} \left[\frac{x + iy}{l'_0} - l'_0 \left(\frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) \right] \\ b^+ &= \frac{1}{2} \left[\frac{x - iy}{l'_0} - l'_0 \left(\frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) \right]. \end{aligned} \quad (22)$$

The eigenenergies labeled by n_{\pm} and σ are

$$\begin{aligned} \varepsilon_{n_+, n_-, \sigma} &= \varepsilon_+ \left(n_+ + \frac{1}{2} \right) \\ &+ \varepsilon_- \left(n_- + \frac{1}{2} \right) + \frac{3\pi N e^2}{4\varepsilon R}, \end{aligned} \quad (23)$$

where $\varepsilon_{\pm} = \hbar\Omega'_0 \pm \alpha\sigma$.

3.2. Many-electron ground state

The ground state energy of the system in terms of the N lowest Hartree eigenenergies ε_i , with i standing for the composite index $[n, m, \sigma]$, reads

$$\mathcal{E}_0 = \sum_{i=1}^N \varepsilon_i - \frac{e^2}{2\varepsilon} \int d\mathbf{r} \int d\mathbf{r}' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (24)$$

where the subtracted integral represents the direct Coulomb energy of the system, counted twice in the summation of the Hartree energies ε_i . Introducing the Fermi energy ε_F separating the occupied and unoccupied Hartree energy levels in the ground state, and calculating the self-interaction integral we arrive at the formula

$$\mathcal{E}_0 = \sum_i \Theta(\varepsilon_F - \varepsilon_i) \varepsilon_i - \frac{3\pi N^2 e^2}{10\varepsilon R}. \quad (25)$$

In the above Θ is the Heaviside function. The Fermi energy is determined by imposing the fixed number of electrons N :

$$N = \sum_i \Theta(\varepsilon_F - \varepsilon_i). \quad (26)$$

The details of calculating the Hartree energy \mathcal{E}_0 are given in Appendix A, and here we shall only present the final result:

$$\mathcal{E}_0 = \frac{9\pi N^2 e^2}{20\varepsilon R} + \frac{2}{3} N^{3/2} \hbar\Omega'_0 \sqrt{1 - \frac{\beta^2 N}{36}}. \quad (27)$$

The radius of the dot R can now be determined from the minimum condition $\partial\mathcal{E}_0/\partial R = 0$, equivalent to the equation

$$\omega_0^2 = \frac{3\pi N e^2}{4\varepsilon R^3 m^*} \left[1 - \frac{100a_B}{27\pi R} \left(1 - \frac{\beta^2 N}{36} \right) \right], \quad (28)$$

where $a_B = \varepsilon\hbar^2/m^*e^2$ is the effective Bohr radius. Confining our considerations to the case of the large number of electrons, we can solve the above equation perturbatively with respect to the small parameter $a_B/R \ll 1$. The zeroth order approximation R_0 can be written in the form

$$R_0^3 = \frac{3\pi N e^2}{4\varepsilon m^* \omega_0^2} \quad (29)$$

and coincides with the classical result obtained in Ref. [21]. Assuming the first-order approximation in the form $R = R_0(1 + \delta)$, the correction δ reads

$$\delta = \frac{100a_B}{81\pi R_0} \left(1 - \frac{\beta^2 N}{36} \right). \quad (30)$$

Disregarding higher corrections (non-linear in δ), the effective confining frequency Ω'_0 can be found based on its definition (14):

$$\Omega_0'^2 = \Omega_0^2 \left(1 - \frac{\beta^2 N}{36} \right), \quad (31)$$

where we use the notation

$$\Omega_0^2 = \frac{100a_B}{27\pi R_0} \omega_0^2. \quad (32)$$

Finally, we arrive at the formula for the ground state energy in the Hartree approximation:

$$\mathcal{E}_0 = \frac{9\pi N^2 e^2}{20\varepsilon R_0} + \frac{1}{3} \hbar\Omega_0 \left(1 - \frac{\beta^2 N}{36} \right) N^{3/2}. \quad (33)$$

The first term in the above equation, calculated in Ref. [21], is the classical energy of N interacting electrons confined in a parabolic well:

$$\begin{aligned} \frac{9\pi N^2 e^2}{20\varepsilon R_0} &= \int d\mathbf{r} n(\mathbf{r}) \cdot \frac{1}{2} m^* \omega_0^2 r^2 \\ &+ \frac{e^2}{2\varepsilon} \int d\mathbf{r} \int d\mathbf{r}' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \end{aligned} \quad (34)$$

The second term is the quantum correction and splits into the energy of oscillation with the frequency Ω_0 :

$$\frac{1}{3}\hbar\Omega_0 N^{3/2} = \sum_i \Theta(\varepsilon_F - \varepsilon_i) \frac{1}{2} m^* \Omega_0^2 \langle i | r^2 | i \rangle \quad (35)$$

and the spin-orbit interaction term.

Let us now include perturbatively the exchange interaction, neglected so far in the Hartree approximation. As the first-order correction $\Delta\mathcal{E}$ we shall calculate the average value of the exchange operator G , defined by Eq. (9), in the Hartree ground state obtained without including the spin-orbit interaction:

$$\Delta\mathcal{E} = \sum_i \Theta(\varepsilon_F - \varepsilon_i) \langle i | G_i | i \rangle |_{\beta=0}. \quad (36)$$

We have verified that the effect due to the spin-orbit interaction is indeed negligible here: for $\beta = 0.3$ the correction to $\Delta\mathcal{E}$ does not exceed 0.15 meV per electron for $N < 100$ (compare with the energy scale in Fig. 1). Similarly, the second-order correction proved to be smaller than the first-order correction by the orders of magnitude (reaching merely 10^{-2} meV), which is then a good approximation to the actual exchange energy.

As shown in Appendix C, Eq. (36) can be conveniently written as

$$\Delta\mathcal{E} = -\frac{4\sqrt{5}}{9\sqrt{3}} \left(1 - \frac{3}{4\sqrt{N}} \right) \frac{N^{7/4} e^2}{\varepsilon R_0} (1 - \delta_0), \quad (37)$$

where $\delta_0 = \delta(\beta = 0)$.

Thus we have obtained the total ground state energy \mathcal{E} of the system of N electrons confined in a parabolic well, including the kinetic energy, the direct and exchange Coulomb interaction, and the spin-orbit coupling:

$$\mathcal{E} = \mathcal{E}_0 + \Delta\mathcal{E}. \quad (38)$$

In Fig. 1 we present the average ground state energy per electron $\varepsilon = \mathcal{E}/N$ plotted as a function of the number of electrons N . The two curves corresponding to the parameter β equal 0.3 and 0.6 are shown to be a reasonable interpolation between the classical result by Shikin et al. [21] and the experimental data by Ashoori et al. [6].

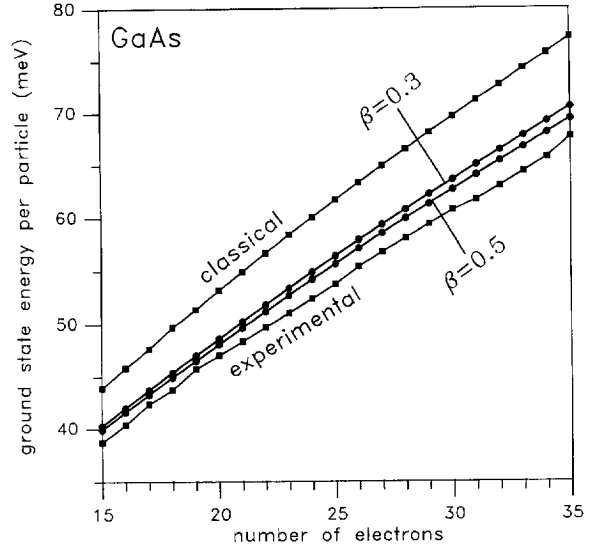


Fig. 1. The average ground state energy per electron as a function of the number of electrons in the dot. The classical result (squares) is taken from Ref. [21], the experimental data (squares) – from Ref. [4], and the two curves in between (circles) are obtained within our model for two values of the spin-orbit coupling constant β (GaAs, $\hbar\omega_0 = 5.4$ meV).

3.3. Far infrared absorption

Let us now consider the selection rules for the optical transitions of the system under the far infra-red (FIR) radiation. Absorption of the FIR light, leading to the excitation of the electron droplet, has been a powerful tool in the experimental studies of quantum dots [2–5].

Since the wavelength of the FIR light is much larger than the radius of the dot, one can use the dipole approximation for describing the interaction between the light and electrons. The probability of the optical transition between the initial (i) and final (f) states is proportional to the squared matrix element of this interaction:

$$d_{fi}^2 \sim \left| \left\langle f \left| e\mathbf{E} \cdot \sum_i \Theta(\varepsilon_F - \varepsilon_i) \mathbf{r}_i \right| i \right\rangle \right|^2, \quad (39)$$

where \mathbf{E} is the electric field, uniform over the volume of the dot. The dipole matrix element d_{fi} vanishes unless there is a pair of the HF states, one in the initial and the other in the final many-electron state, with

equal spins and different by unity in each of the orbital quantum numbers $[n, m]$:

$$\sigma^f = \sigma^i, \quad |n^f - n^i| = 1, \quad |m^f - m^i| = 1, \quad (40)$$

with all other corresponding HF states equal in the initial and final state. In other words, the absorption of a FIR photon leads to the excitation of a single electron from its (initial) HF state to another (final) HF state with the same spin σ and the orbital quantum numbers changed according to Eq. (40). Translating these selection rules to the Fock–Darwin representation we have

$$\begin{aligned} \sigma^f &= \sigma^i, & n_+^f &= n_+^i \pm 1, & n_-^f &= n_-^i, \\ \text{or} & & & & & \\ \sigma^f &= \sigma^i, & n_-^f &= n_-^i \pm 1, & n_+^f &= n_+^i, \end{aligned} \quad (41)$$

i.e. the excited electron changes one of its orbital quantum numbers $[n_+, n_-]$ by unity.

The above selection rules lead to the splitting of the resonance energy:

$$\mathcal{E}^f - \mathcal{E}^i = \varepsilon_{\pm} = \hbar\Omega'_0 \pm \frac{1}{2}\alpha. \quad (42)$$

The magnitude of this splitting α depends on the number of electrons according to Eq. (B.5).

4. Quantum dot in a magnetic field

4.1. Single-electron states

Sketched in the previous section for the case of zero magnetic field the procedure of minimization of the Hartree energy with respect to the dot radius R , with later perturbative inclusion of the exchange interaction, has been also carried out for non-zero fields. The explicit form of the Hartree equations including the presence of a perpendicular magnetic field is

$$\begin{aligned} \left(-\frac{\hbar^2}{2m^*} \Delta + \frac{1}{2}m^* \left(\Omega_B'^2 + \frac{1}{4}\omega_c^2 \right) r^2 - \frac{1}{2}\hbar\omega_c l \right. \\ \left. - g\mu_B \sigma B + \alpha l \sigma \right) \psi_i(\mathbf{r}\sigma) = \left(\varepsilon_i - \frac{3\pi N e^2}{4\epsilon R(B)} \right) \psi_i(\mathbf{r}\sigma), \end{aligned} \quad (43)$$

where $\omega_c = eB/m^*c$ is the effective cyclotron frequency and the zero field radius R appearing in the definition of Ω_B' (14) is now replaced by $R(B)$. We

shall also denote the total confining frequency by $\Omega'^2 = \Omega_B'^2 + \frac{1}{4}\omega_c^2$, and its corresponding characteristic length by $l = \sqrt{\hbar/m^*\Omega'}$.

The eigenfunctions of Eq. (43) are of the same form as given by Eqs. (15) and (20), only with the characteristic length replaced by l . The corresponding eigenenergies read

$$\begin{aligned} \varepsilon_{nm\sigma} &= \hbar\Omega'(n+1) - \frac{1}{2}\hbar\omega_c m \\ &\quad - g\mu_B \sigma B + \alpha m \sigma + \frac{3\pi N e^2}{4\epsilon R(B)}, \end{aligned} \quad (44)$$

or, in the other representation,

$$\begin{aligned} \varepsilon_{n_+n_-\sigma} &= \varepsilon_+ \left(n_+ + \frac{1}{2} \right) + \varepsilon_- \left(n_- + \frac{1}{2} \right) \\ &\quad - g\mu_B \sigma B + \frac{3\pi N e^2}{4\epsilon R}, \end{aligned} \quad (45)$$

with $\varepsilon_{\pm} = \Omega'_0 \pm (\frac{1}{2}\hbar\omega_c + \alpha\sigma)$. Since the Zeeman splitting is rather small for GaAs ($g \sim \frac{1}{2}$ yielding $g\mu_B \sim 0.05$ meV/T), which is the most common material used for the quantum dots, we shall neglect it in the further considerations.

Including the magnetic field leads to the possibility of crossings between different energy levels ε_i . Whether the two close levels ε_1 and ε_2 actually cross, or their crossing is forbidden, depends on vanishing of the off-diagonal matrix element of the operator describing the change of the Hamiltonian due to small change of the field. Thus the condition for the allowed level-crossing is

$$\left\langle 1 \left| \frac{\partial H}{\partial B} \right| 2 \right\rangle \equiv 0. \quad (46)$$

The operator $\partial H/\partial B$ commutes with the spin and inversion ($\mathbf{r} \rightarrow -\mathbf{r}$) operators. Its commutation with the angular momentum requires assumed here circular symmetry of the confining potential. Hence, while for the states of non-equal quantum numbers n and σ we have the condition (46) guaranteed, for a pair of states different only in m in general it is no longer true. This leads to the anti-crossing of levels, which can be taken into account by changing the formulae for eigenenergies:

$$\varepsilon_{nm\sigma} = \hbar\Omega'(n+1) + m \left| \frac{1}{2}\hbar\omega_c + \alpha\sigma \right| + \frac{3\pi N e^2}{4\epsilon R(B)}. \quad (47)$$

Analogously we have to modify the definition of a pair of energies ε_+ and ε_- , appearing in Eq. (45), into $\varepsilon_{\pm} = \Omega'_0 \pm |\frac{1}{2}\hbar\omega_c + \alpha\sigma|$. Let us underline that this rearrangement of levels is a perturbative approximation, beyond the Hartree–Fock approach.

4.2. Many-electron ground state

The many-electron Hartree ground state in the magnetic field $\mathcal{E}_0(B)$ is defined analogously as in Eq. (24). Using the procedure sketched in Appendix D one can bring it to the form

$$\mathcal{E}_0(B) = \frac{9\pi N^2 e^2}{20\varepsilon R_0} + \frac{2}{3} N^{2/3} \hbar \times \left(\omega_0^2 u_B - \frac{3\pi N e^2}{4\pi m^* R(B)^3} \right)^{1/2} \sqrt{1 - \frac{\beta^2 f_B^2 N}{36}}, \quad (48)$$

with the functions f_B and u_B defined in Appendix D by Eqs. (D.16) and (D.17), respectively.

Analogously as for the zero magnetic field, the ground state radius of the dot $R(B)$ can be found from the minimum energy condition

$$\frac{\partial \mathcal{E}_0(B)}{\partial R(B)} = 0 \quad (49)$$

which resolves into the equation

$$\omega_0^2 u_B = \frac{3\pi N e^2}{4\pi m^* R(B)^3} \left[1 + \frac{100 a_B}{27\pi R(B)} \left(1 - \frac{\beta^2 f_B^2 N}{36} \right) \right]. \quad (50)$$

In the zeroth order approximation we obtain

$$R_0(B)^3 = \frac{3\pi N e^2}{4\pi m^* \omega_0^2 u_B} = \frac{1}{u_B} R_0^3. \quad (51)$$

where R_0 is given by Eq. (29). The first order correction $\delta(B)$ defined as: $R(B) = R_0(B)(1 + \delta(B))$ reads

$$\delta(B) = \frac{100 a_B}{81\pi R_0(B)} \left(1 - \frac{\beta^2 f_B^2 N}{36} \right). \quad (52)$$

In Fig. 2 we have drawn the radius as a function of the field. The dependence is fairly weak. When the magnetic field is increased, at low fields the radius also increases, and later, at higher fields, slightly falls down. The initial increase of the radius in the rising

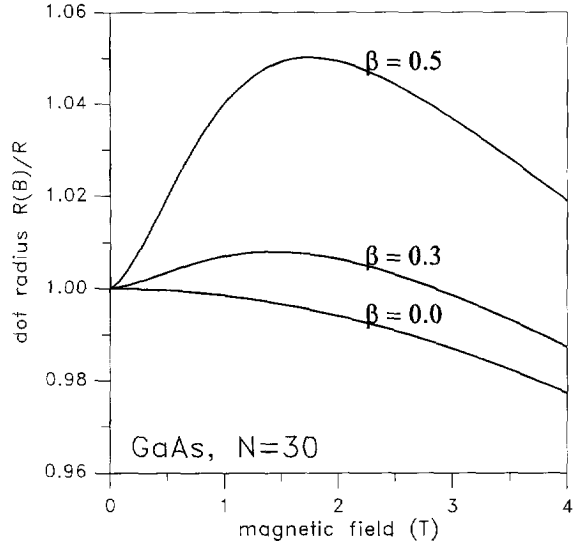


Fig. 2. The dot radius as a function of the magnetic field for $N = 30$ electrons. The three curves correspond to the spin–orbit coupling constant β equal to 0.0, 0.3 and 0.5 (GaAs, $\hbar\omega_0 = 5.4$ meV).

field is an effect due to the spin–orbit interaction, and vanishes for $\beta = 0$.

Finally, the ground state energy in the Hartree approximation can be found in the form

$$\mathcal{E}_0(B) = \frac{9\pi N^2 e^2}{20\varepsilon R_0(B)} + \frac{1}{3} u_B^{2/3} \hbar \Omega_0 \left(1 - \frac{\beta^2 f_B^2 N}{36} \right) N^{3/2}. \quad (53)$$

Calculating the correction due to the exchange energy in the obtained above Hartree ground state is far more complicated for non-zero magnetic fields. Therefore the hypothesis is used, according to which the kind of dependence of the exchange energy on the number of particles is not affected by the presence of the field [22]. As a result we obtain the following formula for the exchange energy:

$$\Delta \mathcal{E}(B) = -\frac{4\sqrt{5}}{9\sqrt{3}} \left(1 - \frac{3}{4\sqrt{N}} \right) \frac{N^{7/4} e^2}{\varepsilon R_0(B)} (1 - \delta_0(B)), \quad (54)$$

where $\delta_0(B) = \delta(B; \beta = 0)$. Thus the total ground state energy within our approach reads

$$\mathcal{E}(B) = \mathcal{E}_0(B) + \Delta \mathcal{E}(B), \quad (55)$$

and the average energy per particle is $\varepsilon(B) = \mathcal{E}(B)/N$.

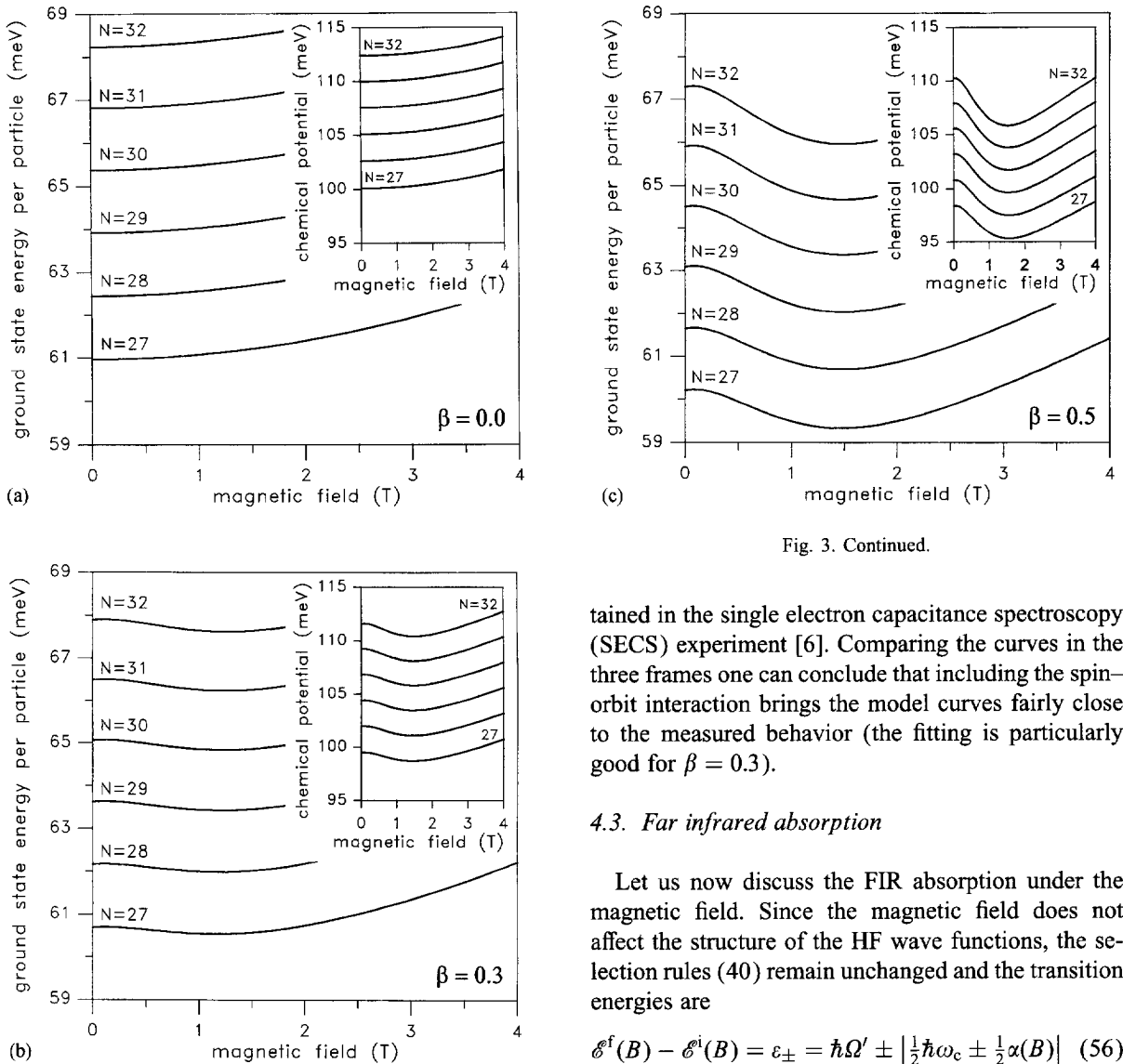


Fig. 3. Continued.

Fig. 3. The average ground state energy per electron as a function of the magnetic field and the number of electrons. The three frames correspond to the spin-orbit coupling constant β equal to 0.0, 0.3 and 0.5 (GaAs, $\hbar\omega_0 = 5.4$ meV). Insets show the chemical potentials.

In Fig. 3 we drew the magnetic field evolution of the average ground state energy per electron $\varepsilon(B) = \mathcal{E}(B)/N$. The three frames correspond to the parameter β equal 0.0 (no spin-orbit coupling), 0.3 and 0.6. We find the qualitative agreement between our curves and the data reported by Ashoori et al., ob-

tained in the single electron capacitance spectroscopy (SECS) experiment [6]. Comparing the curves in the three frames one can conclude that including the spin-orbit interaction brings the model curves fairly close to the measured behavior (the fitting is particularly good for $\beta = 0.3$).

4.3. Far infrared absorption

Let us now discuss the FIR absorption under the magnetic field. Since the magnetic field does not affect the structure of the HF wave functions, the selection rules (40) remain unchanged and the transition energies are

$$\mathcal{E}^f(B) - \mathcal{E}^i(B) = \varepsilon_{\pm} = \hbar\Omega' \pm \left| \frac{1}{2}\hbar\omega_c \pm \frac{1}{2}\alpha(B) \right| \quad (56)$$

and we deal with four resonance branches.

In Fig. 4 we compare the dependence of the FIR resonance energies obtained within our model with that reported by Demel et al. [4]. Assuming that the experimentally observed higher mode is due to the spin-orbit interaction as presented here, we again managed to find a good agreement for $\beta = 0.3$. Particularly, the zero-field lower resonance energy (~ 2.8 meV), the magnetic field at which the anti-crossing occurs (~ 1 T), and the energy at this crossing (~ 3.9 meV), seem to be fit very well. A gap separating the anti-crossing levels, observed in the

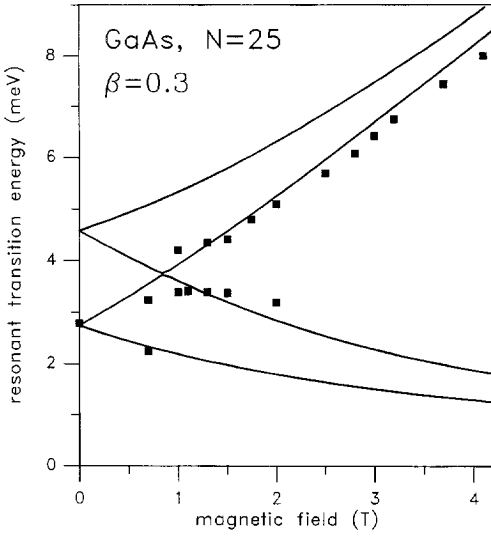


Fig. 4. FIR absorption spectra of a quantum dot containing 25 electrons. Squares – experiment by Demel et al. [4], lines – the model (GaAs, $\beta = 0.3$, $\hbar\omega_0 = 7.5$ meV).

experiment, is probably due to a slight anisotropy of the confining potential.

5. Conclusions

The self-consistent theory of a many-electron quantum dot has been developed with the inclusion of the electron–electron (Coulomb) and spin–orbit interactions. Included here quantum corrections to the ground state energy of the system improve the classical result by Shikin et al. [21] and compare well with the experiments by Demel et al. [4] and Ashoori et al [6]. The spin–orbit interaction is shown to have a strong effect on the electronic structure of the system, leading to the splitting of the resonance energy in the far infrared (FIR) absorption. Predicted here anti-crossing of the FIR absorption modes in the magnetic field describes very well the similar behavior reported by Demel et al. [4].

The critical magnetic field, at which the FIR modes cross and a bump in the ground state energy occurs, is around 1 T, which agrees with the experiments for GaAs [4, 6], and on the other hand with the numerical calculations for a two-electron InSb dot by Darnhofer and Rössler [19].

Acknowledgements

The work was supported by the KBN grants PB 674/P03/96/10 and PB 1152/P03/94/06. We also wish to thank Dr. Pawel Hawrylak (IMS NRC Ottawa) for useful discussions and comments.

Appendix A. Hartree energy at zero magnetic field

In order to perform the summations over the occupied states in Eqs. (25) and (26), it is convenient to introduce the non-zero temperature of the electrons T , and eventually find the limit for $T \rightarrow 0$. The temperature leads to a replacement of the sharp Heaviside function in Eqs. (25) and (26) by the smooth Fermi distribution function:

$$n_s(\varepsilon_+ n_+ + \varepsilon_- n_-) = \left(1 + \exp \frac{\varepsilon_+ n_+ + \varepsilon_- n_- - \mu_s}{k_B T} \right)^{-1}, \quad (\text{A.1})$$

where $\mu_s = \mu - \frac{1}{2}(\varepsilon_+ + \varepsilon_-)$ and μ is the chemical potential.

In order to conveniently hide for the moment the constant terms in Eqs. (23) and (25) we introduce the primed energy symbol

$$\mathcal{E}' = \mathcal{E} - N \cdot \frac{3\pi N e^2}{4\epsilon R} + \frac{3\pi N e^2}{10\epsilon R} = \mathcal{E} + \frac{9\pi N e^2}{20\epsilon R} \quad (\text{A.2})$$

and rewrite Eqs. (25) and (26) in the form

$$N = \sum_{n_+, n_-, \sigma} n_s(\varepsilon_+ n_+ + \varepsilon_- n_-), \quad (\text{A.3})$$

$$\begin{aligned} \mathcal{E}'(T) = & \sum_{n_+, n_-, \sigma} (\varepsilon_+ n_+ + \varepsilon_- n_-) \\ & \times n_s(\varepsilon_+ n_+ + \varepsilon_- n_-) + N \frac{1}{2}(\varepsilon_+ + \varepsilon_-). \end{aligned} \quad (\text{A.4})$$

In order to find the thermodynamically stable state we shall further introduce the following thermodynamical potential:

$$\Phi = \sum_{n_+, n_-, \sigma} \phi_s(\varepsilon_+ n_+ + \varepsilon_- n_-), \quad (\text{A.5})$$

where we define: $\phi_s(\varepsilon) = -k_B T \ln(1 + \exp[(\mu_s - \varepsilon)/(k_B T)])$. At low temperatures the minimization procedure with respect to Φ is equivalent to finding the ground state, as we have

$$\mathcal{E}'(T) = \Phi + \mu N - TS \tag{A.6}$$

(with the entropy $S = \partial\Phi/\partial T$) and

$$\mathcal{E}'_0 = \Phi_0 + \varepsilon_F N, \tag{A.7}$$

where: $\Phi_0 = \lim_{T \rightarrow 0} \Phi$ and $\varepsilon_F = \lim_{T \rightarrow 0} \mu$.

Let us now introduce the Laplace transformations

$$\begin{aligned} n_s(\varepsilon) &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dp \tilde{n}_s(p) e^{p\varepsilon}, \\ \tilde{n}_s(p) &= \int_0^\infty d\varepsilon n_s(\varepsilon) e^{-\varepsilon p}, \\ \phi_s(\varepsilon) &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dp \tilde{\phi}_s(p) e^{p\varepsilon}, \\ \tilde{\phi}_s(p) &= \int_0^\infty d\varepsilon \phi_s(\varepsilon) e^{-\varepsilon p}. \end{aligned} \tag{A.8}$$

Using these expressions we can rewrite Eqs. (A.3) and (A.4) as follows:

$$N = \sum_\sigma \int_0^\infty d\varepsilon z_0(\varepsilon) \left(-\frac{\partial n_s}{\partial \varepsilon} \right), \tag{A.9}$$

$$\Phi = \sum_\sigma \int_0^\infty d\varepsilon z_1(\varepsilon) \left(-\frac{\partial n_s}{\partial \varepsilon} \right), \tag{A.10}$$

where

$$z_0(\varepsilon) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dp \frac{e^{p\varepsilon}}{p(1 - e^{-p\varepsilon_+})(1 - e^{-p\varepsilon_-})}, \tag{A.11}$$

$$z_1(\varepsilon) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dp \frac{e^{p\varepsilon}}{p^2(1 - e^{-p\varepsilon_+})(1 - e^{-p\varepsilon_-})}. \tag{A.12}$$

We chose the constant c in such a way that all the singular points of the subintegral lie on the left-hand side of the integral contour (the contour encloses all singularities inside). Since $-\partial n_s/\partial \varepsilon$ tends to the Dirac's

delta for $T \rightarrow 0$, one finds that:

$$\begin{aligned} N &= \frac{1}{2} \sum_\sigma \left\{ \left[\frac{\mu_{0s}^2}{\varepsilon_+ \varepsilon_-} + \mu_{0s} \left(\frac{1}{\varepsilon_+} + \frac{1}{\varepsilon_-} \right) + \frac{1}{2} \right] \right. \\ &\quad + \left[P_1 \left(\frac{\mu_{0s}}{\varepsilon_+} \right) + P_1 \left(\frac{\mu_{0s}}{\varepsilon_-} \right) \right] \\ &\quad - \frac{\varepsilon_+}{\varepsilon_-} \left[P_2 \left(\frac{\mu_{0s}}{\varepsilon_+} \right) - \frac{1}{12} \right] \\ &\quad \left. - 2 \frac{\varepsilon_-}{\varepsilon_+} \left[P_2 \left(\frac{\mu_{0s}}{\varepsilon_-} \right) - \frac{1}{12} \right] + 2F_0 \left(\frac{\mu_{0s}}{\varepsilon_+}, \frac{\mu_{0s}}{\varepsilon_-} \right) \right\}, \end{aligned} \tag{A.13}$$

where $\mu_{0s} = \varepsilon_F - \frac{1}{2}(\varepsilon_+ + \varepsilon_-)$, and

$$\begin{aligned} \Phi_0 &= -\frac{1}{6} \sum_\sigma \left\{ \varepsilon_F \left[\frac{\mu_{0s}^2}{\varepsilon_+ \varepsilon_-} + \mu_{0s} \left(\frac{1}{\varepsilon_+} + \frac{1}{\varepsilon_-} \right) + \frac{1}{2} \right] \right. \\ &\quad - 3 \left[\varepsilon_+ P_2 \left(\frac{\mu_{0s}}{\varepsilon_+} \right) + \varepsilon_- P_2 \left(\frac{\mu_{0s}}{\varepsilon_-} \right) \right] \\ &\quad - 6 \left[\frac{\varepsilon_+^2}{\varepsilon_-} P_3 \left(\frac{\mu_{0s}}{\varepsilon_+} \right) + \frac{\varepsilon_-^2}{\varepsilon_+} P_3 \left(\frac{\mu_{0s}}{\varepsilon_-} \right) \right] \\ &\quad \left. - 6\sqrt{\varepsilon_+ \varepsilon_-} F_1 \left(\frac{\mu_{0s}}{\varepsilon_+}, \frac{\mu_{0s}}{\varepsilon_-} \right) \right\}. \end{aligned} \tag{A.14}$$

In the above formulae we have introduced the following notation:

$$P_{2j}(x) = \sum_{i=1}^\infty \frac{\cos(2\pi i x)}{2^{2j-1} i^{2j} \pi^{2j}},$$

$$P_{2j+1}(x) = \sum_{i=1}^\infty \frac{\sin(2\pi i x)}{2^{2j} i^{2j+1} \pi^{2j+1}},$$

$$F_0(x, y) = -\frac{\varepsilon_+ \varepsilon_-}{\pi^2} \sum_{i,j=1}^\infty \frac{\cos(2\pi i x) - \cos(2\pi j y)}{(i\varepsilon_-)^2 - (j\varepsilon_+)^2}$$

$$\begin{aligned} F_1(x, y) &= \frac{\sqrt{\varepsilon_+ \varepsilon_-}}{\pi^2} \sum_{i,j=1}^\infty \\ &\quad \times \frac{(\varepsilon_+/(2\pi i)) \sin(2\pi i x) - (\varepsilon_-/(2\pi j)) \sin(2\pi j y)}{(i\varepsilon_-)^2 - (j\varepsilon_+)^2}. \end{aligned} \tag{A.15}$$

The above functions are periodic with the period 1. In the relevant range of domain the absolute value of each function is less than unity. Moreover, note that

for $0 < x < 1$

$$P_1(x) \simeq -x + \frac{1}{2} \rightarrow |P_1(x)| \leq \frac{1}{2},$$

$$P_2(x) \simeq \frac{1}{2}x^2 - \frac{1}{2}x + \frac{1}{12} \rightarrow |P_2(x)| \leq \frac{1}{12},$$

$$P_3(x) \simeq \frac{1}{6}x^3 - \frac{1}{4}x^2 + \frac{1}{12}x \rightarrow |P_3(x)| \leq 0.009. \tag{A.16}$$

The energy of the system \mathcal{E}'_0 one can find from Eq. (A.14) using $\varepsilon_F(N)$ determined from Eq. (A.13). Taking into account that $\varepsilon_{\pm} = \Omega'_0 \pm \alpha\sigma$ and introducing: $v_F = \varepsilon_F/\sqrt{\varepsilon_+\varepsilon_-}$, Eq. (A.13) can be rewritten as follows:

$$\begin{aligned} N + \frac{1}{2} \frac{(\hbar\Omega'_0)^2 + (\alpha_0/2)^2}{(\hbar\Omega'_0)^2 - (\alpha_0/2)^2} \\ = v_F^2 + \frac{1}{2} \sum_{\sigma} \left\{ \left[P_1 \left(\frac{\mu_{0s}}{\varepsilon_+} \right) + P_1 \left(\frac{\mu_{0s}}{\varepsilon_-} \right) \right] \right. \\ \left. - 2 \frac{\varepsilon_+}{\varepsilon_-} \left[P_2 \left(\frac{\mu_{0s}}{\varepsilon_+} \right) - \frac{1}{12} \right] - 2 \frac{\varepsilon_-}{\varepsilon_+} \right. \\ \left. \times \left[P_2 \left(\frac{\mu_{0s}}{\varepsilon_-} \right) - \frac{1}{12} \right] + 2F_0 \left(\frac{\mu_{0s}}{\varepsilon_+}, \frac{\mu_{0s}}{\varepsilon_-} \right) \right\}. \end{aligned} \tag{A.17}$$

The absolute values of all periodic functions are ranged here by unity. Hence, for $N \gg 1$, we note that all the terms under the summation on the right-hand side of the above equation are small compared to N if only

$$\begin{aligned} \left| 2 \frac{\hbar\Omega'_0 + \frac{1}{2}\alpha}{\hbar\Omega'_0 - \frac{1}{2}\alpha} \left[P_2 \left(\frac{\mu_{0s}}{\hbar\Omega'_0 + \alpha/2} \right) - \frac{1}{12} \right] \right| \leq 1 \\ \text{or } \alpha \leq \frac{6}{5} \hbar\Omega'_0. \end{aligned} \tag{A.18}$$

Provided this condition one can use the perturbation method and look for the solution in the form of the following series:

$$v_F = v_{0F} + v_{1F} + v_{2F} + \dots, \tag{A.19}$$

where: $|v_{0F}| \gg |v_{1F}| \gg |v_{2F}| \gg \dots$ From Eq. (A.17) we find

$$v_{0F} = \sqrt{N + \frac{1}{2} \frac{(\hbar\Omega'_0)^2 + (\frac{1}{2}\alpha)^2}{(\hbar\Omega'_0)^2 - (\frac{1}{2}\alpha)^2}} \sim \sqrt{N} \tag{A.20}$$

and, using: $\mu_{0s}^0 = \varepsilon_{0F} - \hbar\Omega'_0 = v_{0F} \sqrt{(\hbar\Omega'_0)^2 - (\frac{1}{2}\alpha)^2} - \hbar\Omega'_0$:

$$\begin{aligned} v_{1F} = -\frac{1}{4v_{0F}} \sum_{\sigma} \left\{ P_1 \left(\frac{\mu_{0s}^0}{\varepsilon_+} \right) + P_1 \left(\frac{\mu_{0s}^0}{\varepsilon_-} \right) \right. \\ \left. + 2F_0 \left(\frac{\mu_{0s}^0}{\varepsilon_+}, \frac{\mu_{0s}^0}{\varepsilon_+} \right) - 2 \frac{\varepsilon_+}{\varepsilon_-} \left[P_2 \left(\frac{\mu_{0s}^0}{\varepsilon_+} \right) - \frac{1}{12} \right] \right. \\ \left. - 2 \frac{\varepsilon_-}{\varepsilon_+} \left[P_2 \left(\frac{\mu_{0s}^0}{\varepsilon_-} \right) - \frac{1}{12} \right] \right\} \sim \frac{1}{\sqrt{N}}. \end{aligned} \tag{A.21}$$

Using the above expressions for v_F we find that (for $N \gg 1$)

$$\varepsilon_F = v_{0F} \sqrt{(\hbar\Omega'_0)^2 - (\frac{1}{2}\alpha)^2} \left[1 + \frac{v_{1F}}{v_{0F}} + O(N^{-3/2}) \right], \tag{A.22}$$

$$\begin{aligned} \Phi_0 = -\frac{N}{3} v_{0F} \sqrt{(\hbar\Omega'_0)^2 - (\frac{1}{2}\alpha)^2} \\ \times \left[1 + 3 \frac{v_{1F}}{v_{0F}} + O(N^{-3/2}) \right], \end{aligned} \tag{A.23}$$

$$\begin{aligned} \mathcal{E}'_0 = \Phi_0 + N\varepsilon_F \\ = \frac{2}{3} N v_{0F} \sqrt{(\hbar\Omega'_0)^2 - (\frac{1}{2}\alpha)^2} [1 + O(N^{-3/2})]. \end{aligned} \tag{A.24}$$

The main non-oscillating term in the above formula for Φ_0 is of the order of $N\sqrt{N}$ while the oscillating terms are at most of the order of \sqrt{N} . In the formula for \mathcal{E}'_0 the non-oscillating term is of the order of $N\sqrt{N}$ and the oscillating terms are at most of the order of unity.

The estimation of the magnitude of spin-orbit coupling constant α is given in Appendix B. Using Eq. (B.5), the final form of the formula for the Hartree energy, given explicitly in Eq. (27), can be now obtained from Eq. (A.24) by substituting Eq. (B.5) and shifting \mathcal{E}'_0 back by the previously omitted constant (according to Eq. A.2).

Appendix B. Spin-orbit coupling constant at zero magnetic field

According to Eq. (2) one needs to estimate the average self-consistent field $\langle \delta U \rangle$ acting on an

electron. The energy of a classical particle in the two-dimensional potential $\frac{1}{2}m^*\Omega_0'^2 r^2$, moving on the orbit of radius r , is

$$\delta U = \frac{1}{2}m^*\Omega_0'^2 r^2 + \frac{1}{2}\Omega_0' l. \quad (\text{B.1})$$

Substituting the classical variables by the respective operators and averaging δU first over the quantum state $[n, m, \sigma]$,

$$\langle nm\sigma | \delta U | nm\sigma \rangle = \frac{1}{2}\hbar\Omega_0'(n+m+1) \quad (\text{B.2})$$

and then over all occupied states, one can obtain the following formula:

$$\langle \delta U \rangle = \frac{1}{2N}\hbar\Omega_0' \sum_{nm\sigma} (n+m+1)n_s(n\hbar\Omega_0'), \quad (\text{B.3})$$

where the spin-orbit energy under the distribution function n_s has been neglected. One can now use the following relation:

$$\begin{aligned} & \sum_{nm\sigma} (n+m+1)n_s(nx+my) \\ &= \left(\frac{\partial \Phi_0}{\partial x} \right)_{x=\varepsilon_F} + \left(\frac{\partial \Phi_0}{\partial y} \right)_{y=\varepsilon_F}, \end{aligned} \quad (\text{B.4})$$

and finally arrive at the formula:

$$\alpha = \frac{1}{3}\beta\hbar\Omega_0'\sqrt{N}. \quad (\text{B.5})$$

Based on the above equation, the second criterion in Eq. (A.18) can be expressed as

$$\sqrt{N} < \frac{18}{5\beta}, \quad (\text{B.6})$$

which gives $N < 144$ for $\beta = 0.3$.

Appendix C. Fock energy at zero magnetic field

Eq. (36) can be written as

$$\Delta \mathcal{E} = -\frac{2e^2}{\varepsilon} \sum_{n,n'} \sum_{m,m'}' I_{nm}^{n'm'} n_{0s}(n\hbar\Omega_0) n_{0s}(n'\hbar\Omega_0), \quad (\text{C.1})$$

where the prime in the second sum excludes terms with $m = m'$, and

$$\begin{aligned} I_{n,m}^{n'm'} &= \int d\mathbf{r} \int d\mathbf{r}' \frac{\psi_{nm}^*(\mathbf{r})\psi_{n'm'}(\mathbf{r})\psi_{n'm'}^*(\mathbf{r}')\psi_{nm}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \\ &= \frac{1}{l_0'} \int_0^\infty dx x \int_0^\infty dx' x \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i(m-m')\theta} \\ &\quad \times \frac{R_{nm}(x)R_{n'm'}(x)R_{nm}(x')R_{n'm'}(x')}{\sqrt{x^2 - 2xx' \cos \theta + x'^2}}. \end{aligned} \quad (\text{C.2})$$

Expanding the subintegral into the Legendre polynomials and integrating over θ one obtains

$$\begin{aligned} I_{n,m}^{n'm'} &= \frac{1}{l_0'} \int_0^\infty dx x^2 R_{nm}(x)R_{n'm'}(x) \\ &\quad \times \left\{ \int_0^1 dt t R_{nm}(tx)R_{n'm'}(tx) t^{|\Delta m|} \right. \\ &\quad \times \sum_{k=0}^\infty t^{2k} a_{k+|\Delta m|} a_k \\ &\quad \left. + \int_1^\infty dt R_{nm}(tx)R_{n'm'}(tx) t^{-|\Delta m|} \right. \\ &\quad \left. \times \sum_{k=0}^\infty t^{-2k} a_{k+|\Delta m|} a_k \right\}, \end{aligned} \quad (\text{C.3})$$

where $\Delta m = m - m'$ and $a_k = (2k-1)!!/(2k)!!$. The integral $I_{n,m}^{n'm'}$ decays rapidly for $\Delta m \rightarrow \infty$ and hence we can cut off the summation over m' in Eq. (C.1) keeping only the terms with $m' = m \pm 1$. In the integral over x we deal with a subintegral with factor e^{-x^2} and thus the most contributes the region around $x = 1$. Provided that the function in braces (in Eq. (C.3)) is smooth with respect to x , it can be replaced by its value at $x = 1$. Moreover, since $R_{nm}(t)R_{n'm'}(t) \sim e^{-t^2}$ the second term in the braces can be neglected as small in comparison with the first one. Hence, for $|\Delta m| = 1$ the integral $I_{n,m}^{n'm'}$ attains the form:

$$\begin{aligned} I_{n,m}^{n'm'} &\simeq \frac{1}{l_0'} \int_0^\infty dx x^2 R_{nm}(x)R_{n'm'}(x) \\ &\quad \times \int_0^1 dt t^2 R_{nm}(t)R_{n'm'}(t) \left(\frac{1}{2} + \frac{3}{16}t^2 + \dots \right) \\ &\simeq \frac{1}{3l_0'} \left(\int_0^\infty dx x^2 R_{nm}(x)R_{n'm'}(x) \right)^2, \end{aligned} \quad (\text{C.4})$$

where we have taken into account the relation

$$\int_0^1 dt t^2 R_{nm}(t) R_{n'm'}(t) \simeq \frac{2}{3} \int_0^\infty dt t^2 R_{nm}(t) R_{n'm'}(t). \quad (\text{C.5})$$

Since

$$\int_0^\infty dx x^2 R_{nm}(x) R_{n'm\pm 1}(x) = \pm \frac{m}{|m|} \left[\sqrt{1 + \frac{n \pm m}{2}} \delta_{n', n+1} - \sqrt{\frac{n \mp m}{2}} \delta_{n', n-1} \right], \quad (\text{C.6})$$

we have

$$I_{nm, n'm\pm 1} = \frac{1}{3l'_0} \left[\left(1 + \frac{n \pm m}{2} \right) \delta_{n', n+1} + \left(\frac{n \mp m}{2} \right) \delta_{n', n-1} \right], \quad (\text{C.7})$$

and

$$\begin{aligned} \Delta \mathcal{E} &= -\frac{2e^2}{\epsilon l'_0} \sum_{nm, n'm'} n_{0s}(n\hbar\Omega_0) n_{0s}(n'\hbar\Omega_0) \\ &\quad \times (I_{nm, n'm-1} \delta_{m', m-1} + I_{nm, n'm+1} \delta_{m', m+1}) \\ &= -\frac{4e^2}{3\epsilon l'_0} \left[\sum_{nm} (n+1) n_{0s}(n\hbar\Omega_0) - \frac{N}{4} - \frac{1}{2} \right]. \end{aligned} \quad (\text{C.8})$$

Using Eq. (B.4) we finally find the correction due to exchange interaction in the form of Eq. (37).

Appendix D. Hartree energy in a magnetic field

Similarly as in the case of the zero magnetic field (see Appendix A) it is convenient to shift the Hartree energy $\mathcal{E}_0(B)$ and introduce

$$\mathcal{E}'_0(B) = \mathcal{E}_0(B) - \frac{9\pi N^2 e^2}{20\epsilon R(B)}, \quad (\text{D.1})$$

given by

$$\begin{aligned} \mathcal{E}'_0(B) &= \sum_{n_+ n_- \sigma} (\epsilon_+ n_+ + \epsilon_- n_-) n_s(\epsilon_+ n_+ + \epsilon_- n_-) \\ &\quad + N \frac{1}{2} (\epsilon_+ + \epsilon_-). \end{aligned} \quad (\text{D.2})$$

In order to calculate $\mathcal{E}'_0(B)$ we further introduce the notation:

$$\begin{aligned} v_F^2 &= \epsilon_F^2 \frac{(\hbar\Omega'_B)^2 - (\frac{1}{2}\alpha(B))^2}{[(\hbar\Omega'_B)^2 - (\frac{1}{2}\alpha(B))^2]^2 - (\frac{1}{2}\hbar\omega_c\alpha(B))^2} \quad (\text{D.3}) \\ \zeta^2 &= \frac{[(\hbar\Omega'_B)^2 - (\frac{1}{2}\alpha(B))^2] \cdot [(\hbar\Omega'_B)^2 - (\frac{1}{2}\hbar\omega_c)^2]}{[(\hbar\Omega'_B)^2 - (\frac{1}{2}\alpha(B))^2]^2 - (\frac{1}{2}\hbar\omega_c\alpha(B))^2} \end{aligned} \quad (\text{D.4})$$

and rewrite Eq. (A.13) as

$$\begin{aligned} N - \frac{1}{2} + \zeta^2 &= v_F^2 + \frac{1}{2} \sum_{\sigma} \left\{ \left[P_1 \left(\frac{\mu_{0s}}{\epsilon_+} \right) + P_1 \left(\frac{\mu_{0s}}{\epsilon_-} \right) \right] \right. \\ &\quad + 2F_0 \left(\frac{\mu_{0s}}{\epsilon_+}, \frac{\mu_{0s}}{\epsilon_-} \right) \\ &\quad \left. - 2 \frac{\epsilon_+}{\epsilon_-} \left[P_2 \left(\frac{\mu_{0s}}{\epsilon_+} \right) - \frac{1}{12} \right] \right. \\ &\quad \left. - 2 \frac{\epsilon_-}{\epsilon_+} \left[P_2 \left(\frac{\mu_{0s}}{\epsilon_-} \right) - \frac{1}{12} \right] \right\}. \end{aligned} \quad (\text{D.5})$$

All the oscillating functions here are small compared to N if

$$\left| 2 \frac{\epsilon_+}{\epsilon_-} \left[P_2 \left(\frac{\mu_{0s}}{\epsilon_+} \right) - \frac{1}{12} \right] \right| \ll N \quad (\text{D.6})$$

or

$$\begin{aligned} &\left| \sqrt{(\hbar\Omega'_B)^2 + (\frac{1}{2}\hbar\omega_c)^2} + \frac{1}{2}\hbar\omega_c \right| \left| 1 + 2 \frac{\alpha(B)\sigma}{\hbar\omega_c} \right| \\ &\ll 4N \left[\sqrt{(\hbar\Omega'_B)^2 + (\frac{1}{2}\hbar\omega_c)^2} \right. \\ &\quad \left. - \frac{1}{2}\hbar\omega_c \left| 1 + 2 \frac{\alpha(B)\sigma}{\hbar\omega_c} \right| \right]. \end{aligned} \quad (\text{D.7})$$

At low magnetic fields, i.e. for $\frac{1}{2}\hbar\omega_c \ll \alpha(B)$, the corrections to Ω' and α due to the field are negligible and the above condition is satisfied for sufficiently high N . At strong magnetic fields, when $\frac{1}{2}\hbar\omega_c \gg \alpha(B)$, it takes

the form

$$\sqrt{1 + \left(\frac{\omega_c}{2\Omega'_B}\right)^2} + \frac{\omega_c}{2\Omega'_B} \ll 4N \left[\sqrt{1 + \left(\frac{\omega_c}{2\Omega'_B}\right)^2} - \frac{\omega_c}{2\Omega'_B} \right], \quad (\text{D.8})$$

which leads to

$$\left(\frac{\omega_c}{2\Omega'_B}\right)^2 \ll N. \quad (\text{D.9})$$

For example, taking the parameters for GaAs and $N = 15$ the above yields $B \ll 17$ T. The solution of Eq. (D.5) can be represented as the series: $v_F = v_{0F} + v_{1F} + \dots$, where

$$v_{0F} = \sqrt{N - \frac{1}{2} + \zeta^2}. \quad (\text{D.10})$$

The first-order correction we find as

$$v_{1F} = -\frac{1}{4v_{0F}} \sum_{\sigma} \left\{ \left[P_1 \left(\frac{\mu_{0s}^{\sigma}}{\varepsilon_+} \right) + P_1 \left(\frac{\mu_{0s}^{\sigma}}{\varepsilon_-} \right) \right] + 2F_0 \left(\frac{\mu_{0s}^{\sigma}}{\varepsilon_+}, \frac{\mu_{0s}^{\sigma}}{\varepsilon_-} \right) - 2\frac{\varepsilon_+}{\varepsilon_-} \left[P_2 \left(\frac{\mu_{0s}^{\sigma}}{\varepsilon_+} \right) - \frac{1}{12} \right] - 2\frac{\varepsilon_-}{\varepsilon_+} \left[P_2 \left(\frac{\mu_{0s}^{\sigma}}{\varepsilon_-} \right) - \frac{1}{12} \right] \right\}, \quad (\text{D.11})$$

where $\mu_{0s}^{\sigma} = \varepsilon_{0F} - \hbar\Omega$. Using the above expressions for v_F , we obtain

$$\varepsilon_F = v_{0F} \sqrt{\frac{[(\hbar\Omega'_B)^2 - (\frac{1}{2}\alpha(B))^2]^2 - (\frac{1}{2}\hbar\omega_c\alpha(B))^2}{(\hbar\Omega'_B)^2 - (\frac{1}{2}\alpha(B))^2}} \times \left[1 + \frac{v_{1F}}{v_{0F}} + O(N^{-3/2}) \right] \quad (\text{D.12})$$

$$\varepsilon'_0(B) = \frac{2}{3}Nv_{0F} \times \sqrt{\frac{[(\hbar\Omega'_B)^2 - (\frac{1}{2}\alpha(B))^2]^2 - (\frac{1}{2}\hbar\omega_c\alpha(B))^2}{(\hbar\Omega'_B)^2 - (\frac{1}{2}\alpha(B))^2}} \times [1 + O(N^{-3/2})]. \quad (\text{D.13})$$

Following the similar procedure as for the zero magnetic field (see Appendix B) we shall now estimate

spin-orbit coupling constant, which is now a function of the field. Analogously to Eq. (B.3) we have (neglecting here the spin-orbit energy):

$$\langle \delta U \rangle = \frac{1}{2N} \hbar\Omega'_B \frac{\Omega'_B}{\Omega} \sum_{nm\sigma} (n+m+1)n_s \times (n\hbar\Omega + \frac{1}{2}m\hbar\omega_c), \quad (\text{D.14})$$

and further

$$\alpha(B) = \frac{1}{3}f_B\hbar\Omega'_B\sqrt{N}, \quad (\text{D.15})$$

with the renormalizing function

$$f_B = \sqrt{1+z^2/N} \left(1 - \frac{z}{\sqrt{1+z^2}} \right) \Big|_{z=\omega_c/2\Omega'_B}. \quad (\text{D.16})$$

At low fields the function f_B tends to unity, while for $B \rightarrow \infty$ it decays to zero: $f_B \sim 1/\sqrt{N}$. Therefore, to a good approximation, in the definition of f_B we can replace Ω'_B by Ω_0 , defined by Eq. (32).

Finally, using the above formula for $\alpha(B)$, and introducing the following function u_B :

$$u_B = 1 + (\omega_c/2\Omega_0)^2 \frac{1}{1-z} \times \left(\frac{1}{N} - 4\frac{z}{(1-z)} \right) \Big|_{z=\beta^2 f_B^2 N/36}, \quad (\text{D.17})$$

the Hartree energy of the system can be written in the form of Eq. (48).

References

- [1] For the reviews and references see T. Chakraborty, Comments Condens. Matter Phys. 16 (1992) 35.
- [2] D. Heitmann, Physica B 212 (1995) 201.
- [3] J. Alsmeyer, E. Batke and J.P. Kotthaus, Phys. Rev. B 41 (1990) 1699.
- [4] T. Demel, D. Heitmann, P. Grambow and K. Ploog, Phys. Rev. Lett. 64 (1990) 788.
- [5] B. Meurer, D. Heitmann and K. Ploog, Phys. Rev. Lett. 68 (1992) 1371.
- [6] R.C. Ashoori, H.L. Stormer, J.S. Weiner, L.N. Pfeiffer, K.W. Baldwin and K.W. West, Phys. Rev. Lett. 71 (1993) 613.
- [7] M. Bayer, A. Schmidt, A. Forchel, F. Faller, T.L. Reinecke, P.A. Knipp, A.A. Dremin and V.D. Kulakovskii, Phys. Rev. Lett. 74 (1995) 3439.
- [8] K. Brunner, U. Bockelmann, G. Abstreiter, M. Walther, G. Böhm, G. Tränkle and G. Weimann, Phys. Rev. Lett. 69 (1992) 3216.

- [9] P.M. Petroff and S.P. Denbaars, *Superlattices Microstruct.* 15 (1994) 15.
- [10] S. Raymond, S. Fafard, P.J. Poole, A. Wójs, P. Hawrylak, S. Charbonneau, D. Leonard, R. Leon, P.M. Petroff and J.L. Merz, *Phys. Rev. B* 54 (1996) 11548.
- [11] A. Kumar, S.E. Laux and F. Stern, *Phys. Rev. B* 42 (1990) 5166.
- [12] A. Wójs, P. Hawrylak, S. Fafard and L. Jacak, *Phys. Rev. B* 54 (1996) 5604.
- [13] A. Wójs and P. Hawrylak, *Phys. Rev. B* 53 (1996) 10 841.
- [14] W. Kohn, *Phys. Rev.* 123 (1961) 1242.
- [15] P. Maksym and T. Chakraborty, *Phys. Rev. Lett.* 65 (1990) 108.
- [16] P. Hawrylak and D. Pfannkuche, *Phys. Rev. Lett.* 70 (1993) 485.
- [17] P. Hawrylak, *Phys. Rev. Lett.* 71 (1993) 3347.
- [18] P. Hawrylak, A. Wójs and J.A. Brum, *Solid State Commun.* 98 (1996) 847.
- [19] T. Darnhofer and U. Rössler, *Phys. Rev. B* 47 (1993) 16 020.
- [20] J.J. Palacios, L. Martin-Moreno, G. Chiappe, E. Louis, C. Tejedor, *Phys. Rev. B* 50 (1994) 5760.
- [21] V. Shikin, S. Nazin, D. Heitmann and T. Demel, *Phys. Rev. B* 43 (1991) 11 903.
- [22] S.V. Vonsovskij, *Magnetism* (Nauka, Moscow, 1971; in Russian).