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LETTER TO THE EDITOR

Ground state spin oscillations of a two-electron quantum dot in a magnetic field

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Abstract. Crossings between spin-singlet and spin-triplet lowest states are analysed within the model of a two-electron quantum dot in a perpendicular magnetic field. The explicit expressions in terms of the magnetic field, the magnetic quantum number m of the state and the dimensionless dot size for these crossings are found.

Recent progress in nanostructure technology allows us to thoroughly investigate a quantum motion of confined electrons in semiconductors, in particular, in quantum dots [1,2]. Since the size of a quantum dot as well as the number of electrons is controlled, we can study different correlation effects in the 'artificial atom'. Two interacting electrons in an external potential turn out to be a useful system, providing a basis for understanding the contribution of different components of an effective mean field. A detailed examination of the electron spectrum of a quantum dot can also be approached with alteration of the magnetic field [3].

Low-lying energy levels of a two-dimensional two-electron system in a perpendicular magnetic field have been analysed quantitatively for various confining potentials [4–6]. In particular, for a parabolic confining potential the estimations for singlet–triplet and triplet–triplet ground state phase transitions have been found in the perturbation approach in the limit of the strong magnetic field [4]. The energy spectrum of two interacting electrons in the parabolic confining potential has been obtained analytically for particular values of the magnetic field [7]. In this letter we present the analytical expressions for fulfilment of such phase transitions at arbitrary values of the magnetic field for a parabolic quantum dot.

Our analysis is based on the oscillator representation method (ORM) developed in [8]. The application of this method to calculate the energy spectrum of the two-electron system in the magnetic field is discussed in [9] where the reader can find all necessary details. We consider the two-dimensional version of the model Hamiltonian [9]

$$H = \sum_{j=1}^{2} \left\{ \frac{1}{2m^\star} \left(\vec{p}_j - \frac{e}{c} \vec{A}_j \right)^2 + \frac{m^\star}{2} \left[\omega_0^2 \left(x_j^2 + y_j^2 \right) + \omega_z^2 z_j^2 \right] \right\} + \frac{e^2}{4\pi\epsilon\epsilon_0} \frac{1}{|\vec{r}_1 - \vec{r}_2|} + H_{spin} \qquad (1)$$

assuming $z = 0$. Here $H_{spin} = g\,(\vec{s}_1 + \vec{s}_2)\,\vec{B}$ and $m^\star$ is the effective electron mass. Below, we use the units ($e = c = 1$). For the perpendicular magnetic field ($\vec{B}||z$) we choose a gauge described by the vector

$$\vec{A} = \left[\vec{B} \times \vec{r} \right] /2 = \frac{1}{2} \vec{B}(-y, x, 0).$$

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By introducing the relative and centre-of-mass coordinates $\vec{r} = \vec{r}_2 - \vec{r}_1$, $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$, the Hamiltonian, equation (1), can be separated into the centre-of-mass (CM) and relative-motion (RM) terms

$$H = 2H_q + \frac{1}{2}H_Q + H_{spin} \tag{2}$$

$$H_q = \frac{1}{2}\left[\vec{p}_q + \vec{A}_q\right]^2 + \frac{\overline{h}^2}{2}{\omega_q}^2\rho_q^2 + \frac{k\sqrt{\hbar\omega_0}}{2\rho_q} \tag{3}$$

$$H_Q = \frac{1}{2}\left[\vec{P}_Q + \vec{A}_Q\right]^2 + \frac{\overline{h}^2}{2}{\omega_Q}^2\rho_Q^2 \tag{4}$$

where

$$\omega_Q = 2\omega_0$$
$$\omega_q = \frac{1}{2}\omega_0$$
$$\vec{A}_Q = \vec{A}(q_1) + \vec{A}(q_2)$$
$$\vec{A}_q = \frac{1}{2}(\vec{A}(q_2) - \vec{A}(q_1))$$
$$\vec{A}(q) = \frac{\overline{h}}{m^\star}\left[\vec{B} \times \vec{q}\right].$$

Here we use the variables

$$\vec{q} = \frac{\sqrt{m^\star}}{\overline{h}}\vec{r}$$
$$\vec{Q} = \frac{\sqrt{m^\star}}{\overline{h}}\vec{R}$$
$$\rho_q = \sqrt{q_x^2 + q_y^2}$$

and define the characteristic lengths: the effective radius

$$a^\star = a_B\epsilon\frac{m_e}{m^\star}\left(a_B = 4\pi\epsilon_0\frac{\overline{h}^2}{m_e e^2}\right)$$

and the oscillator length

$$l_0 = (\overline{h}/m^\star\omega_0)^{1/2}.$$

These units allow one to define the dimensionless dot size $k = l_0/a^\star$ [4]. At $k = 0$, we have the model of noninteracting electrons in the magnetic field [10] (see also [3]). The separability and the conservation of the angular momentum lead to a natural ansatz for the eigenfunction of the Hamiltonian, equation (2), i.e. $\Psi = \psi(\vec{q})\,\phi\left(\vec{Q}\right)\chi(\vec{s}_1, \vec{s}_2)$. According to the Pauli principle, if the spatial part of the total wave function is symmetric (antisymmetric) with respect to the inversion $r \to -r$, χ must be a singlet (triplet) spin state. For the eigenvalues we have

$$E = 2\epsilon_r + \frac{1}{2}E_{N,M} + E_S. \tag{5}$$

Here ϵ_r and $E_{N,M}$ are the eigenvalues of the Hamiltonian of the RM and of the CM motion, respectively. The solution to the CM Hamiltonian H_Q is well known [10] and the energy can be written as

$$E_{N,M} = 2\overline{h}\omega_0\left[(2N + |M| + 1)\sqrt{1 + \frac{t^2}{4}} + \frac{1}{2}Mt\right] \tag{6}$$

where $N = 0, 1, ...$ and $M = 0, \pm 1, ...$ are radial and azimuthal quantum numbers, respectively, and $t = \omega_c/\omega_0$ where $\omega_c = \frac{B}{m^\star}$ is the cyclotron frequency. The spin of the two electrons leads to the additional Zeeman energy

$$E_S = g^\star \mu_B B S_z = \frac{\hbar\omega_0}{4}\left[1 - (-1)^m\right] g^\star \frac{m^\star}{m_e} t. \tag{7}$$

Here, m is a magnetic quantum number corresponding to the RM Hamiltonian and $g^\star$ is the effective Landé factor. For the RM energy we obtain†

$$E^{2d}_{nm} = \epsilon_r = \varepsilon^0_{nm} + \varepsilon^c_{nm} \tag{8}$$

where

$$\begin{aligned} \varepsilon^0_{nm} &= \frac{\hbar\omega_0}{2}\left[\frac{m}{2}t + (1 + |m| + 2n)x^2\left(1 + \frac{t^2}{4}\right)^{1/2}\right] \\ \varepsilon^c_{nm} &= \frac{\hbar\omega_0}{2}\frac{xk}{2\sqrt{2}}\left(1 + \frac{t^2}{4}\right)^{1/4}\left[3\frac{\Gamma\left(\frac{1}{2} + |m|\right)}{\Gamma(1 + |m|)} + 2\langle n|h_I|n\rangle\right]. \end{aligned} \tag{9}$$

The quantity x is determined by the following equation:

$$x^4 + \frac{x^3}{\sqrt{2}}\frac{k}{\left(1 + \frac{t^2}{4}\right)^{1/4}}\frac{\Gamma\left(\frac{1}{2} + |m|\right)}{\Gamma(2 + |m|)} - 1 = 0. \tag{10}$$

In the ORM only the lowest positive solution of equation (10) is interesting. In contrast to the perturbative approach the main term ε^0_{nm}, equation (9), also depends on the Coulomb forces. The interaction modifies the external potential and results in the effective mean field potential for the RM. Notice that in the second term ε^c_{nm} there is a contribution arising due to radial excitations, i.e., the term $\langle n|h_I|n\rangle$ [9]. The matrix element $\langle n|h_I|n\rangle$ provides a basis for calculations of the radial excitations modified by the Coulomb interaction and, according to the rules of the ORM, it has the following form:

$$\langle n|h_I|n\rangle = \frac{3}{4}\frac{\Gamma(d/2 - 1/2)}{\Gamma(d/2)} S_n \tag{11}$$

where

$$\begin{aligned} S_n &= \frac{4\Gamma(1 + n)}{3\sqrt{\pi}} \sum_{k=2}^{2n} \frac{(-1)^k \Gamma(k + 1/2)}{\Gamma(k + d/2)} N_k(n, d) \\ N_k(n, d) &= \sum_{p=0}^{n} \frac{2^{2p-k}\Gamma(k + n - p + d/2)}{(n - p)!(2p - k)!\,((k - p)!)^2} \end{aligned}$$

and $d = 2 + 2|m|$. For particular values of the radial quantum number $n = 0, 1, 2$ we obtain $S_0 = 0$, $S_1 = \frac{2}{d}$, $S_2 = \frac{4}{d(d+2)}\left[d + \frac{19}{8}\right]$, respectively. Our result for the RM energy, equations (8) and (9), corresponds to the perturbation approach in the limit $x \to 1$, $\omega_c \gg \omega_0$ and $n = 0$ (see below).

Owing to the separability of the CM energy and the RM energy, we have only two frequencies from equation (6) for dipole transitions $(NM) \to (N'M')$

$$\omega_\pm = \left[\left(\frac{\omega_c}{2}\right)^2 + \omega_0^2\right]^{1/2} \pm \frac{\omega_c}{2} \tag{12}$$

† We have corrected the misprint; i.e. the factor 2, which is present in the equation for the energy of relative motion in [9], is omitted here.

which are not influenced by the Coulomb interaction. This is a simple example of the consequence of the Kohn theorem [11]. Since the centre-of-mass quantum numbers N, M and the quantum number m are conserved by the Coulomb interaction, the ground state has the quantum numbers $N = 0, M = 0, n = 0$. Comparing the energy with different $m \leqslant 0$, we can define the ground state energy at different values of the magnetic field ω_c/ω_0. While without the Coulomb forces the ground state is always the state with $m = 0$, the Coulomb interaction leads to a sequence of different ground states $m = -1, -2, ...$ which are an alternating sequence of singlet and triplet states. In figure 1 we have plotted the energy of states with different m for different values of $k = l_0/a^*$.

The singlet–triplet ground phase transition (crossing) occurs when the condition $E_{0,m} = E_{0,m-1} (m \leqslant 0)$ is fulfilled, where we have introduced the notation $E_{n,m} = E_S + 2E^{2d}_{n,m}$.

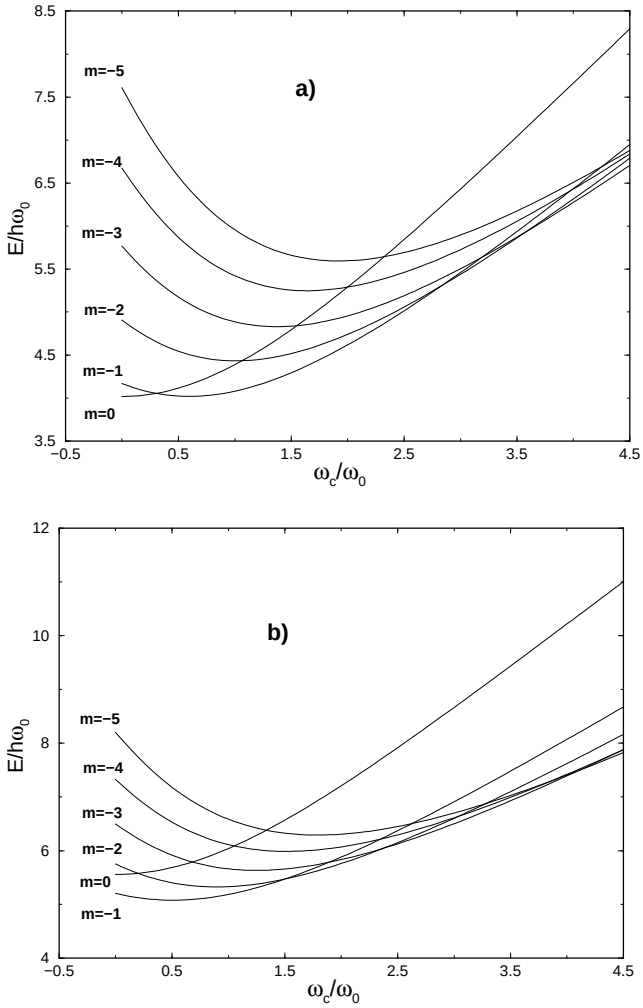

Figure 1. Eigenenergies in units $\hbar\omega_0$ versus the ratio ω_c/ω_0 for a different dot size k. The family of states $N = M = n = 0$ and $m \leqslant 0$ is shown (a) for $k = 2$ and (b) for $k = 4$. As the ratio $k = l_0/a^*$ increases the Coulomb interaction rearranges the sequence of levels.

Taking into account equations (7) and (8), we obtain

$$\frac{\ell_0}{a^*}\Big|_{n=0} = \frac{2\sqrt{2}}{3x}\frac{\Gamma(2+|m|)}{\Gamma(1/2+|m|)}\frac{t}{\left[1+t^2/4\right]^{1/4}}\left[-1+x^2\sqrt{1+\frac{4}{t^2}}+(-1)^m g^*\frac{m^*}{m_e}\right]. \tag{13}$$

We emphasize that this expression is valid at finite values of the magnetic field. Combining equation (10) with equation (13), we can define the value of x at the singlet–triplet crossings $m \to m-1$

$$x = \sqrt{\frac{\sigma t + \sqrt{\left(\sigma^2+\frac{21}{4}\right)t^2+21}}{7\sqrt{1+\frac{1}{4}t^2}}} \tag{14}$$

where

$$\sigma = 1-(-1)^m g^*\frac{m^*}{m_e} = 1-2\beta \qquad \beta = \frac{1}{2}(-1)^m g^*\frac{m^*}{m_e}. \tag{15}$$

Therefore, equations (13) and (14) define the values of the magnetic field which lead to the singlet–triplet crossings in the ground state and also in the excited states of the two-electron system. At the strong magnetic field ($\omega_c \gg \omega_0$) in the lowest order of the parameter β we obtain from equations (13) and (14)

$$x \simeq 1-\frac{1}{5}(-1)^m g^*\frac{m^*}{m_e} \tag{16}$$

$$\frac{\ell_0}{a^*}\Big|_{n=0} = \frac{8}{3}\frac{\Gamma(2+|m|)}{\Gamma(1/2+|m|)}\left[\left(\frac{\omega_0}{\omega_c}\right)^{3/2}+\frac{3}{10}(-1)^m g^*\frac{m^*}{m_e}\left(\frac{\omega_c}{\omega_0}\right)^{1/2}\right]. \tag{17}$$

Equation (17) almost coincides with a similar expression based on the perturbative approach [4] with the exclusion of the coefficient in front of the term arising from the spin contribution.

For the negative Landé factor the spin-splitting energy in the magnetic field will lower the energy of the spin $S_z = +1$ component of the triplet states. In particular, the relation $E_{0,m} = E_{0,m-1} = E_{0,m-2}$ (m odd) defines the point when the singlet phase ceases to exist [4]. Beyond this point we can observe crossings between triplet states defined by the condition $E_{0,m} = E_{0,m-2}$ (m odd), which leads to

$$\frac{\ell_0}{a^*} = \frac{8\sqrt{2}}{3x}\frac{t}{\left[1+t^2/4\right]^{1/4}}\frac{\Gamma(3+|m|)}{\Gamma(1/2+|m|)}\frac{1}{5+4|m|}\left(-1+x^2\sqrt{1+\frac{4}{t^2}}\right). \tag{18}$$

For the triplet–triplet crossings the parameter x can be obtained from equations (13) and (18)

$$x^2 = \frac{4t}{\sqrt{1+t^2/4}}\frac{2+|m|}{47+28|m|}+\sqrt{\frac{16t^2}{1+t^2/4}\frac{(2+|m|)^2}{(47+28|m|)^2}+\frac{3(5+4|m|)}{47+28|m|}}. \tag{19}$$

At the strong magnetic field $\omega_c \gg \omega_0$ for the triplet–triplet crossings $m \to m-2$ (m odd) we obtain the following result:

$$x \simeq 1 \qquad \frac{\ell_0}{a^*} = \frac{8}{3}\frac{\Gamma(3+|m|)}{\Gamma(1/2+|m|)}\frac{1}{5+4|m|}\left(\frac{\omega_0}{\omega_c}\right)^{3/2} \tag{20}$$

which coincides with the estimation of the perturbative approach [4]. The singlet–triplet crossings yield the triplet–triplet ones for polarized electrons. The ground states are determined with odd values of the magnetic quantum number m. The radius of each particular m state decreases as $1/\sqrt{B}$, and the electrons are pushed towards the dot's centre. At very high fields

both the electrons are in the lowest Landau level [12] which, however, consists of the quantum levels given in equations (8) and (9). Naturally, the Pauli principle prevents the occupation of the same quantum state by both the electrons. The Coulomb forces become less important for high-lying single-electron levels. The orbital motion increases the relative distance between electrons weakening the influence of the Coulomb forces on the crossing of levels. The value of the parameter $k = l_0/a^\star$ for the singlet–triplet crossing decreases with increasing the radial quantum number n as well. In particular, for the two-dimensional system we have obtained the following relation between the parameters $k = l_0/a^\star$ for the singlet–triplet crossing at different n

$$\frac{(l_0/a^\star)_{n=1}}{(l_0/a^\star)_{n=0}} = \frac{2+|m|}{7+|m|}. \tag{21}$$

While the interplay between the magnetic field and the Coulomb forces determines the features of the phase transition (singlet $\rightarrow$ triplet) for the ground state ($n = 0$), it is mainly the magnetic field that leads to phase transitions for the high-lying states $n > 0$.

In conclusion, we have found the exact relations between the dimensionless size $k = l_0/a^*$ and the values of the magnetic field for the singlet–triplet and the triplet–triplet crossings in the ground and excited states for two interacting electrons confined by the parabolic potential. The Coulomb interaction is treated exactly within the analytical approach. The spin interaction is important for the singlet–triplet crossings whereas it does not contribute to the triplet–triplet crossings. The last one can be described as the crossing of quantum levels of polarized electrons in the magnetic field.

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