# Energy spectra of two electrons in a harmonic quantum dot

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The laterally confining potential of quantum dots on semiconductors is approximated by a two-dimensional harmonic-oscillator well. The discrete level diagram for two interacting electrons in this potential is calculated in the effective-mass approximation as a function of the dot size and the strength of a magnetic field directed perpendicularly to the dot plane.

Quantum dots in which only a few electrons are bound at semiconductor interfaces have been accomplished recently by advanced technologies.[1] These atomiclike few-electron systems arise when homogeneous two-dimensional electron gases of heterojunctions or metal-oxide-semiconductor (MOS) structures are laterally confined to diameters comparable to the effective Bohr radius of the host semiconductor. Such lateral widths are still much larger than the extensions of the wave functions in the growth direction of the underlying planar semiconductor structure. Hence, quantum dots may be treated as atomiclike disks.

Experimentally, quantum dots have been studied by vertical tunneling,[2] in-plane transport,[3] capacitance versus voltage curves,[4] as well as by far-infrared spectroscopy.[5–7] The descriptions of all these experiments have successfully been based on a harmonic shape of the laterally confining potential, i.e., on a two-dimensional oscillator effective in the plane of the dots. In this Brief Report we calculate the level diagram for two electrons in such a harmonic potential. We fully include the Coulomb interaction and allow for magnetic fields that are applied perpendicular to the plane of the dots. Though this case of two electrons represents the simplest nontrivial problem with regard to the electron number, it has not been treated previously. However, our results can be compared to the ones of the pioneering work of Bryant[8] for two electrons in a quadratic quantum-well box with infinite barriers and to the more recent work of Maksym and Chakraborty[9] who numerically treated three and four electrons in disklike GaAs quantum dots with harmonic confinement potentials.

We proceed in three steps. First, the problem is considered in the absence of a magnetic field taking into account the Coulomb interaction between the two electrons by first-order perturbation theory. This approach provides a good description as long as the dot radius is much less than the effective Bohr radius. It also allows for a straightforward classification of the corresponding states in terms of orbital quantum numbers, total spins, and degeneracies. Subsequently, we numerically calculate the spectra for a wider range of dot sizes. Finally, the Zeeman splittings in magnetic fields of arbitrary strength are included.

We consider two electrons with effective masses $m^*$ in the $z=0$ plane which are confined by a two-dimensional harmonic potential of characteristic frequency $\omega_0$ or length $l_0=(\hbar/m^*\omega_0)^{1/2}$. Their Hamiltonian can be separated into two parts that represent the center of mass and the relative motion, respectively:

$$H=\frac{\mathbf{P}^2}{2M}+\tfrac{1}{2}M\omega_0^2\mathbf{R}^2+\frac{\mathbf{p}^2}{2\mu}+\tfrac{1}{2}\mu\omega_0^2 r^2+\frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{r}\ . \tag{1}$$

Accordingly, we have the center-of-mass coordinates $\mathbf{R}=(\mathbf{r}_1+\mathbf{r}_2)/2$ and $\mathbf{P}=\mathbf{p}_1+\mathbf{p}_2$, and the total mass $M=2m^*$, as well as the relative coordinates $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$ and $\mathbf{p}=(\mathbf{p}_1-\mathbf{p}_2)/2$ and the reduced mass $\mu=m^*/2$. Also, there is the dielectric constant $\epsilon$ of the host semiconductor.[10] The exact eigenfunctions of the center-of-mass motion read

$$\psi(\mathbf{R})=\frac{\sqrt{2}}{l_0}\left[\frac{N!}{\pi(N+|M|)!}\right]^{1/2}e^{iM\varphi}e^{-x^2}x^{|M|}L_N^{|M|}(x^2) \tag{2}$$

with the abbreviation $x=\sqrt{2}\,R/l_0$ and the azimuthal angle $\varphi$.[11] These eigenfunctions and the eigenenergies

$$E_{\text{c.m.}}=(2N+|M|+1)\hbar\omega_0 \tag{3}$$

depend on the radial ($N=0,1,\ldots$) and the azimuthal ($M=0,\pm1,\ldots$) quantum numbers. $L_N^{|M|}$ are generalized Laguerre polynomials.[11] The eigenfunctions and energies for the relative motion are of the same form, if we ignore the Coulomb interaction for the moment, and replace $x=\sqrt{2}R/l_0$ by $r/\sqrt{2}l_0$ as a consequence of the different masses $M$ and $\mu$. For the relative motion we write the quantum numbers with small letters, $n$ and $m$ and so have the energies $E_{n,m}=(2n+|m|+1)\hbar\omega_0$ in zeroth order.

The Coulomb matrix obviously is diagonal with respect to the quantum numbers $N$ and $M$ of the center-of-mass motion. Moreover, it is also diagonal in the angular momentum $m\hbar$. Therefore, we can employ nondegenerate perturbation theory. As a further consequence of the conservation of $m$, we have singlet ($S=0$) and triplet

 

TABLE I. First-order Coulomb energies $E^{(1)}$ for two electrons in a two-dimensional harmonic-oscillator potential. The states are labeled by their degeneracy factor $g$, total spin $S$, as well as by the quantum numbers $(n,m)$ of the relative and $(N,M)$ of the center-of-mass motion. Energies $E^{(0)}$ for the noninteracting electrons are given in units of the oscillator energy $\hbar\omega_0$; first-order Coulomb corrections $E^{(1)}$ in terms of the one of the ground state, namely $(\pi\mathcal{R}^*\hbar\omega_0)^{1/2}$.

| $E^{(0)}$ ($\hbar\omega_0$) | $E^{(1)}$ ($\sqrt{\pi\mathcal{R}^*\hbar\omega_0}$) | $g$ | $S$ | $(n,m)$ | $(N,M)$ |
|---|---|---|---|---|---|
| 2 | 1 | 1 | 0 | (0,0) | (0,0) |
| 3 | $\frac{1}{2}$ | 6 | 1 | (0,±1) | (0,0) |
| | 1 | 2 | 0 | (0,0) | (0,±1) |
| 4 | $\frac{3}{8}$ | 2 | 0 | (0,±2) | (0,0) |
| | $\frac{1}{2}$ | 12 | 1 | (0,±1) | (0,±1) |
| | $\frac{3}{4}$ | 1 | 0 | (1,0) | (0,0) |
| | 1 | 3 | 0 | (0,0) | (1,0)(0,±2) |
| 5 | $\frac{5}{16}$ | 6 | 1 | (0,±3) | (0,0) |
| | $\frac{3}{8}$ | 4 | 0 | (0,±2) | (0,±1) |
| | $\frac{7}{16}$ | 6 | 1 | (1,±1) | (0,0) |
| | $\frac{1}{2}$ | 18 | 1 | (0,±1) | (1,0)(0,±2) |
| | $\frac{3}{4}$ | 2 | 0 | (1,0) | (0,±1) |
| | 1 | 4 | 0 | (0,0) | (1,±1)(0,±3) |

($S=1$) states for even and odd numbers $m$, respectively. Classification of states and analytical results for the Coulomb interaction energy calculated in first order are given in Table I. Note that one can readily formulate dimensionless Coulomb energies in terms of the ratio of oscillator length $l_0$ and effective Bohr radius $a^*$ using the relation $l_0/a^*=(2\mathcal{R}^*/\hbar\omega_0)^{1/2}$.

Perturbation theory is only valid as long as the ratio $l_0/a^*$ is less than unity. At present, this situation can only be realized on InSb ($a^*=67$ nm) whereas on GaAs ($a^*=10$ nm) one typically has quantum dots with values $l_0/a^*\sim 10$. To describe larger dots, we have numerically diagonalized the exact problem, i.e., we take fully into account the Coulomb interaction. Since we use a two-particle wave function, the exchange is included automatically. Typically, for fixed angular momentum $|m|\hbar$ matrices of size $50\times 50$ in the label $n$ are needed to obtain convergent eigenenergies. Numerical problems due to cancellation effects are overcome by an algebraic programming system. The result for lower-lying states is depicted in Fig. 1. It is worth noting that as the dot size increases, the absolute energies decrease roughly proportional to the inverse of the squared oscillator length $l_0^{-2}$. This becomes clear from the inset of Fig. 1 where the ground-state energy is normalized with the Rydberg constant and from the markedly different energy scales in Fig. 2. This figure once more shows the level structure for three distinct values $l_0/a^*$. The arrows indicate the fundamental dipole excitation whose energy is always given by the bare energy $\hbar\omega_0$ in accordance with the generalized Kohn theorem.[9,12]

Most experiments on quantum dots have employed homogeneous magnetic fields **B** perpendicular to the dot

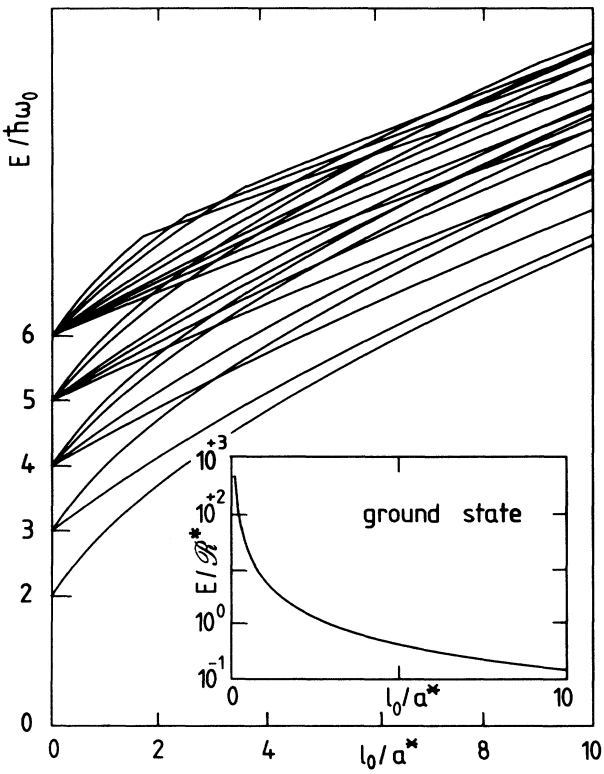


FIG. 1. Lateral eigenenergies for two electrons in a harmonic-oscillator well. The energies are normalized with the oscillator energy $\hbar\omega_0$ and are given vs the ratio of oscillator length $l_0$ and effective Bohr radius $a^*$. The inset shows the ground-state energy in units of the effective Rydberg constant $\mathcal{R}^*$

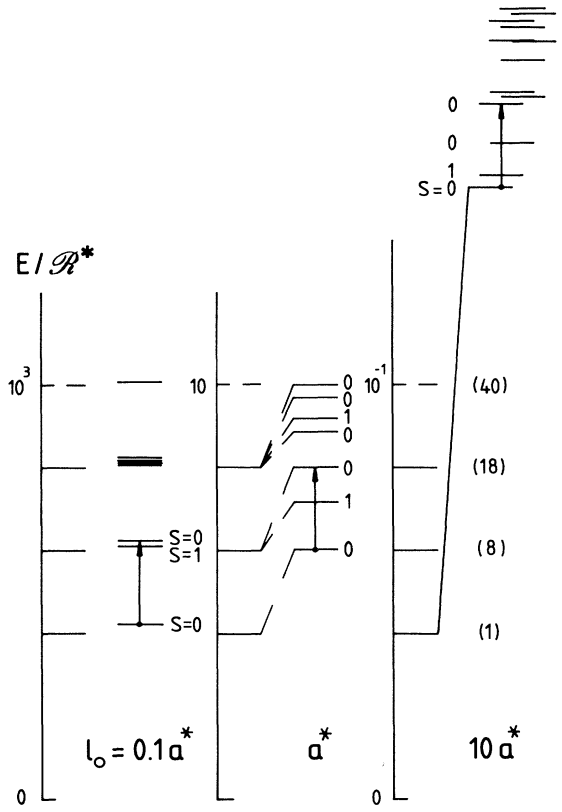


FIG. 2. Spectra for two electrons in harmonic wells of different sizes. Independent particle energies are indicated at the respective energy scales and their degeneracies are given by the numbers in parentheses on the right-hand side. For the largest dot size ($l_0=10a^*$), states of interacting electrons derived from the same independent electron level are equally shifted to the right.

plane. In this case, the Hamiltonian can be separated in the same way as in Eq. (1). In the symmetric gauge of the vector potential $\mathbf{A}$ the exact wave functions of the center-of-mass motion are of the same form as the ones in Eq. (2). The only difference is that we must replace the oscillator length $l_0$ by the characteristic length $L=[\hbar/(\omega_c^2/4+\omega_0^2)^{1/2}m^*]^{1/2}$ with the cyclotron frequency $\omega_c=eB/m^*$. The eigenenergies

$$E_{\text{c.m.}}=(2N+|M|+1)\hbar\left[\left[\frac{\omega_c}{2}\right]^2+\omega_0^2\right]^{1/2}+\frac{\hbar\omega_c}{2}M \qquad (4)$$

of the center-of-mass motion are split according to their angular momenta $M\hbar$. The zeroth-order energies of the relative motion are identical to those of Eq. (4) but again written with small letters $n$ and $m$.

The allowed dipole transitions are rather simple. The dipole operator $2e\mathbf{R}$ only couples to the center-of-mass motion but leaves unchanged the relative motion. The dipole frequencies

$$\omega_{\pm}=\left[\left[\frac{\omega_c}{2}\right]^2+\omega_0^2\right]^{1/2}\pm\frac{\omega_c}{2} \qquad (5)$$

are readily obtained from Eq. (4).[13] Table II summarizes

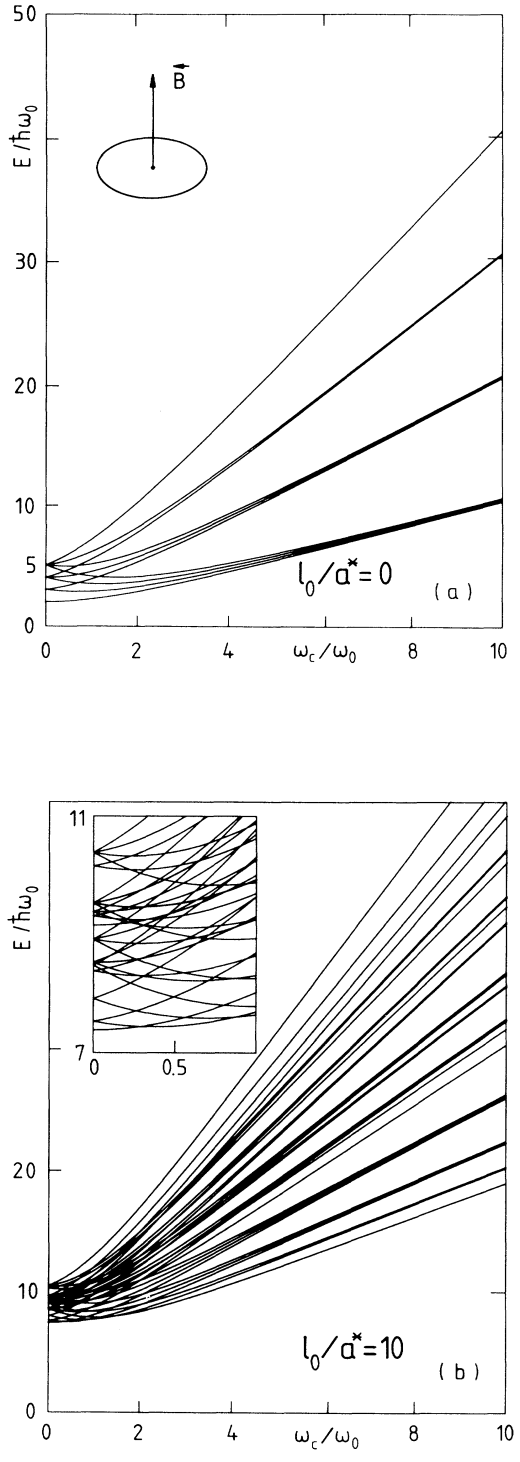


FIG. 3. Zeeman splittings of the eigenenergies for two electrons in a harmonic well. For clarity reasons, only the levels belonging to the four lowest unperturbed states $E^{(0)}$ (see Table I) are depicted. The splittings are calculated (a) for the limit $l_0/a^*=0$ of independent particles and (b) for a larger dot size $l_0/a^*=10$. Away from crossing points there are 10 and 32 energetically different levels, respectively. The inset shows the splittings on enlarged scales in the same units.

TABLE II. Selection rules, matrix elements $D$, and frequencies $\omega$ of dipole transitions $(N,M)\rightarrow(N',M')$ for quantum dots in the harmonic well approximation. The matrix elements are proportional to the length $L=[\hbar/(\omega_c^2/4+\omega_0^2)^{1/2}m^*]^{1/2}$ and the electron number $n_0$. Resonances $\omega_\pm=[(\omega_c/2)^2+\omega_0^2]^{1/2}\pm\omega_c/2$ are excited with the two corresponding circular light polarizations.

| | | $\omega$ | |
|---|---|---|---|
| $(N',\|M'\|)$ | $D$ | $M'\geq 0$ | $M'<0$ |
| $N,\|M\|+1$ | $(N+\|M\|+1)^{1/2}Ln_0$ | $\omega_+$ | $\omega_-$ |
| $N+1,\|M\|-1$ | $(N+1)^{1/2}Ln_0$ | $\omega_-$ | $\omega_+$ |

selection rules and dipole matrix elements and applies for any electron number.

The Coulomb matrix elements in magnetic fields differ from the ones of the zero field case only by the factor $[1+(\omega_c/2\omega_0)^2]^{-1/4}$. In Figs. 3(a) and 3(b) resulting Zeeman splittings are shown. For clarity reasons we omit spin splittings $g^*\mu_B BS_z$ that may be described by an effective Landé factor $g^*$, i.e., we only draw levels with spin components $S_z=0$. In the limit $l_0/a^*=0$ of Fig. 3(a) the Coulomb interaction can be ignored. Then the levels rearrange in increasing magnetic fields in a relatively simple way in order to form Landau states of two independent electrons in infinitely strong fields. At any finite ratio $\omega_c/\omega_0$, however, we have a multitude of Landau-like ladders each of them with the step spacing $\hbar\omega_+$. These ladders are piled up in distances $\hbar\omega_-$ on top of each other. Therefore, the gaps that appear between successive groups of states in Fig. 3(a) only are a consequence of our restriction to the four lowest levels $E^{(0)}$ at $B=0$. In the presence of the Coulomb interaction, the degeneracy of levels is lifted further, as becomes clear from Fig. 3(b). The same spectrum as in Fig. 3(a) is imposed on each particular level of the relative motion described by the quantum numbers $(n,m)$. This results in the rather complex spectrum of Fig. 3(b). Note that the ground state $(n,m,N,M)=(0,m,0,0)$ changes its character $(m=0,-1,-2,\ldots)$ when the strength of the magnetic field increases.

Our analysis provides the simplest explicit example for the generalized Kohn theorem which states that the dipole resonance frequencies of an electron system with harmonic confinement are independent of the electron number as well as of the particular form of the electron-electron interaction.[9,12] The dipole frequencies are always given by the single-particle values $\omega_\pm$ of Eq. (5). The generalized Kohn theorem remains valid in the presence of a magnetic field as long as the spin Hamiltonian is of the simple form presumed above. However, it will be violated when spin-orbit interaction mixes singlet and triplet states. The same is true for conduction-band nonparabolicity with its higher powers of the momentum operator.

To conclude, we have calculated the discrete energy spectra for two electrons in a two-dimensional harmonic well that serves as a simple but suitable model for quantum dots on semiconductor interfaces. The most appealing feature of quantum dots as compared to other atomic-like systems like donors in semiconductors is the tunability of their size and electron number by technological means. Taking this point of view, we have determined the eigenenergies and Zeeman splittings of quantum dot helium as a function of its size.

*Note added in proof.* After the submission of this paper, we became aware of a publication by Kumar, Laux, and Stern,[14] who self-consistently calculated levels of up to more than 10 electrons. They found that a harmonic confinement potential is indeed a very good approximation in real samples.

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