phys. stat. sol. (b) **230**, No. 2, 463–468 (2002)

Stark Effect in Self-Assembled Quantum Dots with Lens Shape

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(Received October 9, 2001; accepted November 30, 2001)

Subject classification: 73.21.La; 73.22.Dj

The electronic states of a self-assembled quantum lens (SAQL) under application of a normal electric field are theoretically investigated for different values of the electric field and lens geometry. Using a conformal analytical image, the lens boundary and the one particle Hamiltonian are mapped into an equivalent operator defined in a semi-spherical boundary. The complete set of solutions for the Stark effect in a quantum lens confined by an infinite barrier is reported. The numerical calculations indicate that the interplay of the lens geometry and the electric field on electrons in the SAQL leads to complicated electron eigenenergies and eigenfunctions. Also, the interactions between states with the same symmetry and anticrossing effects on the energy levels and wavefunctions sharing the same z-angular momentum components are analyzed.

Introduction The interest in quantum dots (QDs) has recently increased due to the novel properties these zero-dimensional structures exhibit as a consequence of spatial confinement [1–6]. Different applications in electro-optical devices [2] make the knowledge of the external electric field influence on the electronic structures important. In the past, the Stark shift in QDs has been theoretically studied in cuboidal nanocrystals [7] and in spherical ones [8–10]. The modern growing techniques have led to the so called self-assembled quantum lens (SAQL) with nearly a lens shape geometry [11–15] characterized by a spherical cap shape of height b and a circular cross section of radius a with $b < a$. Their in-plane radii are typically about 15–100 nm and 3–4 nm height. The present work is devoted to a non-perturbative approach to describe the electronic states in a SAQL under an external electric field normal to its plane assuming a strong confinement regime. Taking advantage of previously reported results [16], the Stark effect in a QD with a lens shape is solved using the conformal transformation method, mapping the effective mass Hamiltonian and the lens domain into an equivalent problem with a semi-spherical contour.

Stark Problem for a Quantum Lens The spatial domain of the SAQL will be denoted by $R_3(a,b)$ and the boundary region by $L_3(a,b)$. The electric field F is taken along the z direction and normal to the SAQL circular cross section. Considering a single particle of effective mass m^* confined inside the dot region, the Schrödinger equation in spherical coordinates leads to the following dimensionless Dirichlet problem:

$$\nabla^2_{\mathbf{r}_1}\Phi(\mathbf{r}_1) + \xi r_1 \cos\theta_1 \Phi(\mathbf{r}_1) + k^2\Phi(\mathbf{r}_1) = 0\,, \tag{1}$$

with $\mathbf{r}_1 \in R_3(a,b)$ and the boundary condition $\Phi(\mathbf{r}_1) = 0$ at $\mathbf{r}_1 \in L_3(a,b)$. Here, $\xi = F/F_0$, $k^2 = E/E_0$, $F_0 = E_0/(|e|a)$, and $E_0 = \hbar^2/(2m^*a^2)$. Due to the axial symmetry

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 0370-1972/02/23004-0463 $ 17.50+.50/0

the solutions of Eq. (1) can be cast as

$$\Phi(r_1, \theta_1, \phi) = \frac{f(r_1, \theta_1)}{\sqrt{r_1} \sin \theta_1} \frac{e^{im\phi}}{\sqrt{2\pi}}\,; \qquad m = 0, \pm 1, \dots, \tag{2}$$

where r_1, θ_1 are plane polar coordinates and $f(r_1, \theta_1)$ satisfies the equation

$$\nabla^2_{r_1,\theta_1} f(r_1, \theta_1) + \left(k^2 - \frac{m^2 - 1/4}{r_1^2 \sin^2 \theta_1} + \xi r_1 \cos \theta_1 \right) f(r_1, \theta_1) = 0 \tag{3}$$

with $f(r_1, \theta_1) = 0$ at $(r_1, \theta_1) \in L_2(a, b)$.

The Dirichlet problem of Eq. (3) in the lens domain $R_2(a, b)$ does not allow explicit analytical solutions. Using the conformal mapping reported in [16], Eq. (3) can be mapped into

$$\nabla^2_{r,\theta} f^{(\beta,\xi)}(r, \theta) + \mathcal{J}_\beta(r, \theta) \left(k^2(\beta, \xi) - \frac{m^2 - 1/4}{\mathcal{X}^2_\beta(r, \theta)} + \xi Z_\beta(r, \theta) \right) f(r, \theta) = 0\,, \tag{4}$$

with boundary conditions $f(a, \theta) = 0$ and $f(r, \pi/2) = 0$ and the new domain is a semicircle of radius a. The parameter β, the Jacobian $\mathcal{J}_\beta$, and the functions $\mathcal{X}^2_\beta$ and Z_β are the mathematical objects which contain the lens geometry information (see Ref. [16]). Equation (4) reduces to Eq. (3) when the semi-spherical case, $b/a = 1$, is recovered. Hence, the function $f^{(\beta,\xi)}(r, \theta)$ can be obtained as an expansion in terms of the complete set of orthonormal eigenfunctions $\{f^{(0)}_{n,l,m}(r, \theta)\}$ (solution of Eq. (4) for $b/a = 1$ at $F = 0$), and given by

$$f^{(0)}_{n,l,m}(r, \theta) = \sqrt{\sin \theta}\, P_l^{|m|}(\cos \theta)\, J_{l+1/2}(\mu_n^{(l)} r)\,; \qquad l = 1, 2, 3 \dots, -l \le m \le l\,, \tag{5}$$

where $\mu_n^{(l)}$ is the n-th zero of the Bessel function $J_{l+1/2}$. The set (5) is a complete set of orthonormal eigenfunctions for the space of solutions of Eq. (4). The boundary condition at $\theta = \pi/2$ leads to the condition $|l - m| = \text{odd}$. Thus,

$$f^{(\beta,\xi)}_{N,m}(r, \theta) = \sum_{i=\{n,l\}}^{\infty} C_i^{(\beta,\xi)}(N, m)\, f^{(0)}_{i,m}(r, \theta)\,, \tag{6}$$

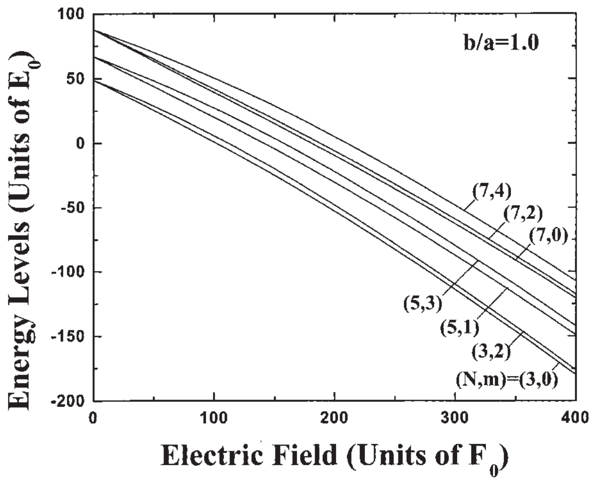

Fig. 1. Exited state energies $E_{N,m}$ of a semi-spherical quantum dot as a function of the electric field. The energies at $F = 0$ correspond to states with angular momentum $l = 3$, 4 and 5. The energy $E_{N,m}$ and the electric field F are given in units of E_0 and F_0, respectively

where i is a certain order of quantum numbers (n, l) and N is a new quantum number. Using Eq. (6) it is possible to show that Eq. (4) is reduced to

$$\sum_i^\infty C_i^{(\beta,\xi)}(N,m)\left\{(\mu_n^{(l)})^2\,\delta_{ij}+(m^2-1/4)\left\langle j\left|\frac{\mathcal{J}_\beta}{\mathcal{X}_\beta^2}-\frac{1}{r^2\sin^2\theta}\right|i\right\rangle\right.$$
$$\left.-\,\xi\langle j|\mathcal{J}_\beta Z_\beta|i\rangle-\;k^2(\beta,\xi)\langle j|\mathcal{J}_\beta|i\rangle\right\}=0\,. \qquad (7)$$

Equation (7) is a generalized eigenvalue problem of infinite order. k^2 are the eigenvalues and $C_i(N,m)$ the eigensolutions. To evaluate numerically the eigenvalues k^2, the

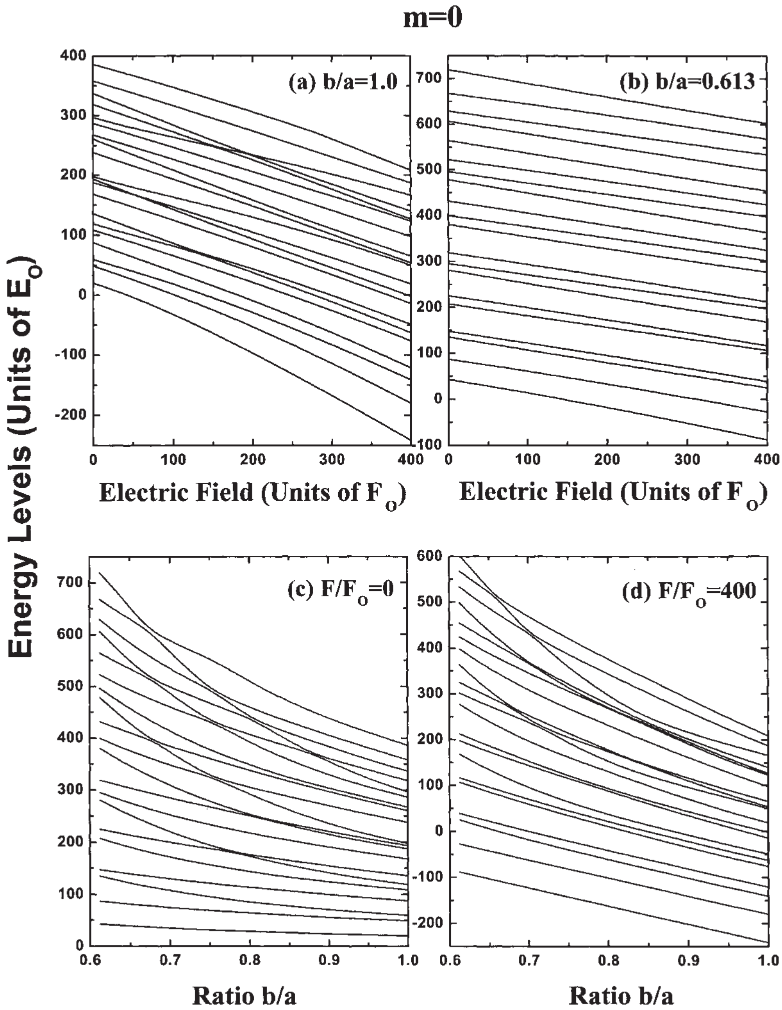

Fig. 2. First 20 energy levels of SAQL as a function of the electric field, for (a) $b/a=1$ and (b) $b/a=0.613$. In part (c) $F/F_0=0$ and in (d) $F/F_0=400$ are shown as a function of the ratio b/a. The energy and the electric field are given in units of E_0 and F_0, respectively

first 100 zeros $\mu_n^{(l)}$ of Bessel functions are sorted for a given value of the quantum number m. A 100 × 100 matrix is enough to obtain a good accuracy for the first 20 eigenvalues. In Fig. 1 the energy levels are plotted as a function of the electric field for the first three degenerated states l = 3, 4, and 5 at $F = 0$ in the semi-spherical case ($b/a = 1$). For $F \neq 0$ the degeneracy is broken as a consequence of the uniaxial direction introduced by the electric field upon the electron motion inside the semi-spherical dot. As the degeneracy is broken for a given state N, the larger m values present the higher energies, and the corresponding slope of the energy levels at $F = 0$ is not zero, showing a first order dependence on the electric field. These characteristics are quite different from those obtained in a QD with spherical shape [10].

In Figs. 2(a) and (b) the dependence of the first 20 energy levels on the normalized electric field are compared for two different QDs ($b/a = 1$ and $b/a = 0.613$). Figures 2(c) and (d) show the same eigenenergies as a function of the lens deformation b/a at $F/F_0 = 0$ and 400, respectively. In all the cases the quantum number m is zero. It can be seen that for a fixed value of the ratio b/a, an increase of the electric field produces a decrease of the energy (Figs. 2(a) and (b)). Otherwise, when b/a takes lower values (for a fixed F), the confinement effect will rise the energy levels to higher values, as should be expected (Figs. 2(c) and (d)). The interaction between the levels in Fig. 2 is characterized by an anticrossing effect. Those states with the same quantum number m present the same symmetry properties, while the energy levels with different quantum number m have different spatial symmetry and can cross each other. Nevertheless, as the ratio b/a of the QD takes smaller values the repulsion between levels is diminished. This behavior is clearly shown in Fig. 2(b) where the dependence of the eigenenergies as a function of the applied field follows almost a parallel law. The same can also be said in Fig. 2(d) for the lower levels, where the stronger applied field ($F/F_0 = 400$) reduces the

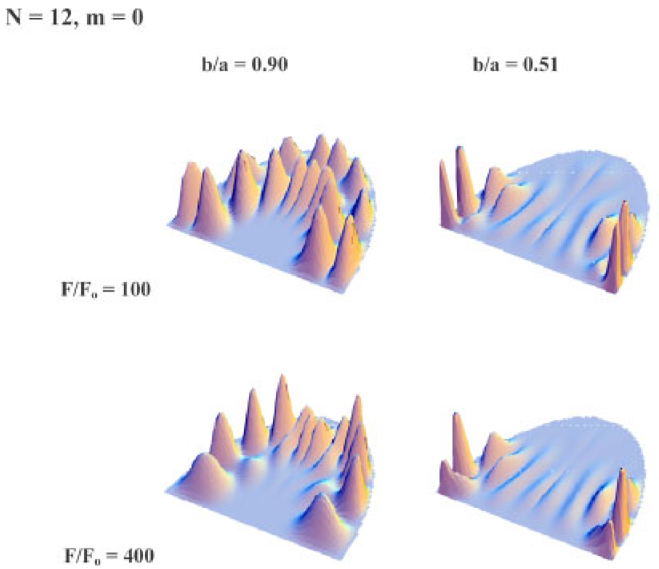

Fig. 3 (online colour). Probability density function of the level $N = 12$, $m = 0$, for two values of the electric field F/F_0 and b/a ratio repulsion interaction between them. Due to the interplay between spatial confinement and electric field in the SAQL, it is not possible to achieve a simple description for the anticrossing effect. The question of a chaotic behavior at different regimes of QD deformation and electric field strength being present or not is beyond the scope of the present paper but will be subject to a future work.

In Fig. 3 the calculated probability density function, $f_{N,m}^{(\beta,\xi)}(r,\theta)\mathcal{J}_{\beta}(r,\theta)$, of the level $N = 12$, $m = 0$ is shown for two values of the electric field and the ratio b/a. It can be seen the change of the nodal distribution due to the effect of the electric field on the carrier. In the case of $b/a = 0.51$ this change is not so strong due to the high confinement in the QL domain, as it was already reported in Fig. 2(b). Our calculations point out that in the case of "flatter" lens the confinement is so strong that the ground level is not affected by the variation of the electric field.

Conclusions The Stark effect and the wavefunctions of a SAQL in an external electric field can be calculated by a generalized variational procedure using a conformal transformation method. It permits to obtain explicitly analytical solutions for the wavefunctions $f_{N,m}^{(\beta,\xi)}(r,\theta)$ given by the expression (6) where the eigenenergies and the coefficients C_i of the problem are obtained by a direct diagonalization of the matrix (7). The levels and their corresponding eigensolutions are studied as functions of lens geometry and applied electric field. The most symmetric case of a semi-sphere at $b/a = 1$ has a constraint $|l - m| =$ odd and a degeneracy at $F = 0$ of order l. These degeneracies are broken by the electric field and lens deformation $b/a < 1$ keeping the two fold degeneracy for $\pm m$ (see Eqs. (2) and (4)). For a given N the lower energy values correspond to lower values of the z-component quantum number. The complex interplay of F and the lens geometry on carriers lead to a complicated electric field dependence of the energy and the wavefunctions in SAQLs. In the case of weak confinement the electric field produces a strong repulsion between levels leading to the anticrossing effect suitable to a complex regime. Finally, the calculation method provides an explicit solution for the Stark effect in SAQLs that can be used to evaluate electro-optical properties of the novel system as a function of its geometrical properties.

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