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LETTER TO THE EDITOR

Exact analytical solutions describing quantum dot, ring and wire wavefunctions

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Abstract

For the first time, exact analytical solutions of electronic wavefunctions in quantum ring-like structures are found using a symmetry-adapted coordinate system. In the case of an infinite potential barrier, it is related to a more general problem of finding resonance modes in a ring-like cavity. The solutions in the parabolic coordinate system are Bessel or confluent hypergeometric functions for quantum dot, ring and wire including objects with flat bases. The continuous evolution from the 0D quantum dot system to the perfect 1D quantum ring system is analysed. The electronic properties (energy levels, wavefunctions and density of states) are continuously followed during the dot to ring transformation until the limit of a perfect 1D quantum ring is reached. The creation of a ring structure by changing the material composition in a dot centre leads to a sharp variation in the energy levels of totally symmetric states. This is a consequence of the immediate build-up of a potential barrier energy in the centre of the ring. Finally the use of the structure of electronic levels to identify the signature of self-organized quantum rings when compared to quantum dots is proposed.

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Recent research developments have been devoted to nano-structured semiconductor materials. Quantum wires (QWs) or quantum dots (QDs) show improved properties as compared to semiconductor quantum wells for high performance optoelectronic devices [1–3]. A remarkable morphological change from dot-like to ring-like of self-assembled quantum dots may occur or be forced during growth [4–6]. It has a great influence on the interband or intraband optical transitions [5] and on optoelectronic device performances based on these structures. The theoretical study of the electronic properties of semiconductor nanostructures

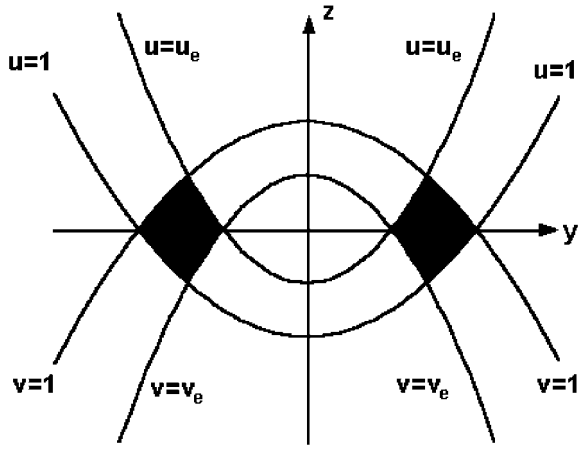

Figure 1. Projection of the parabolic coordinate surfaces in the (y, z) plane. A particular volume is obtained by the boundaries rotated around the z-axis ($0 \leqslant \theta \leqslant 2\pi$). If four orthogonal confocal parabolas are used ($u = u_e$, $v = v_e$, $u = 1$, $v = 1$) a symmetrical ring-shaped volume is obtained. The cross-sections of the ring are represented by the dark surfaces.

can be performed with various sophisticated theoretical schemes. One-band effective mass models have proved, however, to be useful and sufficient for many practical cases [7–10]. In the presence of an infinite potential barrier, the Schrödinger equation is equivalent to the Helmholtz equation [11–14], and the search for solutions is related to a more general problem of finding the resonance modes in a cavity. Various special coordinate sets have been used to reach separable solutions described in the Helmholtz equations [15–19]. Disc-like quantum dots have been described using parabolic coordinates [18, 20], applying the results already known for disc-like cavities [12]. Perfectly asymmetric lens-shaped quantum dots have been analysed using symmetry arguments [18]. We may note that these works are closely related to other works on properties of an atom on the surface of a solid [21] or on the energy spectrum of a hydrogen impurity in a parabolic quantum dot [22]. Various problems may be studied with parabolic coordinates. For example, the Schrödinger equation has already been solved for long range potentials [23, 24].

We first show in this work that the shape, as observed experimentally [4–6], may be continuously changed from dot-like to ring-like using the parabolic coordinates. Analytic solutions are a combination of confluent hypergeometric functions of the first and second kinds or in some particular cases Bessel functions. The transformation of a 0D quantum dot system to a perfect 1D quantum ring system can be continuously described. It is finally shown that an analysis of the structure of electronic levels is used to identify the signature of self-organized quantum rings when compared to quantum dots electronic levels.

The parabolic set of unit-less coordinates (u, v, ϑ) used for the quantum ring is defined by a transformation of Cartesian coordinates ($0 \leqslant u \leqslant \infty$, $0 \leqslant v \leqslant \infty$ and $0 \leqslant \theta \leqslant 2\pi$): $x = auv\cos(\vartheta)$, $y = auv\sin(\vartheta)$ and $z = a(u^2 - v^2)/2$. The theoretical treatment of the quantum ring structure in the parabolic coordinate system (figure 1) has three main advantages. First, a ring may be defined by intersections of the four parabolas ($u = u_e$, $v = v_e$, $u = 1$, $v = 1$) rotated around the z-axis. In figure 1 the cross-sections in the y–z plane of the ring are represented as dark surfaces with a reduced area $S = S_r/a^2$, where S_r is the actual area and a is a parameter of the parabolic metric [12]. For comparison, a wire with the same cross-section is defined from an intersection of the same parabolas in the parabolic cylindrical coordinates

system [11]. We will show in the following that analytical solutions exist in both cases. The limit of the perfect 1D system ($S_r \to 0$ or $u_e \to 1$) is then conveniently obtained both for the wire and the ring. We may note that such a comparison may not be performed for a ring with a circular cross-section. For a toroidal shape, a full variable separation is not possible in the Helmholtz equation [11, 12]. Second, in the limit $u_e \to 0$, the case of the disc or lens-like quantum dot is recovered [12, 18, 20]. The continuous change from a 0D dot system to a ring and then to a perfect 1D system can be studied as a function of the reduced section S. Third, the solutions of electronic states of quantum nanostructures with flat bases are readily obtained by keeping only odd solutions with respect to the horizontal plane symmetry [18].

In the general case (finite potential barrier), the Hamiltonian is only separable in (u, v) and ϑ coordinates, and $\Xi(u, v, \theta) = \chi(u, v)\,\mathrm{e}^{\mathrm{i}n\theta}$ are general solutions of the problem with the Hamiltonian given by the expression

$$H = \frac{-\hbar^2}{2}\vec{\nabla}\frac{1}{m(\vec{r})}\vec{\nabla} + V(\vec{r}) = -\frac{\hbar^2}{2a^2(u^2+v^2)}\left[\frac{1}{u}\frac{\partial}{\partial u}\frac{u}{m_{(u,v)}}\frac{\partial}{\partial u} + \frac{\partial}{\partial v}\frac{v}{m_{(u,v)}}\frac{\partial}{\partial v}\right] - \frac{\hbar^2}{2a^2u^2v^2m_{(u,v)}}\frac{\partial^2}{\partial\theta^2} + V(u, v).$$

In the case of an infinite potential barrier, however, the Hamiltonian is separable in u, v and ϑ coordinates, and the wavefunction appears as a product of functions of independent variables $\Xi(u, v, \theta) = f(u)g(v)\mathrm{e}^{\mathrm{i}m\theta}$. The f and g functions are solutions of two coupled differential equations with a separation constant C:

$$u^2\frac{\mathrm{d}^2 f}{\mathrm{d}u^2} + u\frac{\mathrm{d}f}{\mathrm{d}u} + (Eu^4 - Cu^2 - n^2)f = 0$$

and

$$v^2\frac{\mathrm{d}^2 g}{\mathrm{d}v^2} + v\frac{\mathrm{d}g}{\mathrm{d}v} + (Ev^4 + Cv^2 - n^2)g = 0.$$

Solutions of these equations [13, 14] include confluent hypergeometric functions of the first kind ϕ and second kind ψ:

$$f(u) = F(u, C, E, m) = \mathrm{e}^{-\mathrm{i}\sqrt{E}u^2/2}(\mathrm{i}\sqrt{E}u^2)^{m/2}\begin{pmatrix}\lambda_f\phi\left(\frac{-\mathrm{i}C}{4\sqrt{E}} + \frac{m+1}{2}, m+1, \mathrm{i}\sqrt{E}u^2\right)\\ +\mu_f\psi\left(\frac{-\mathrm{i}C}{4\sqrt{E}} + \frac{m+1}{2}, m+1, \mathrm{i}\sqrt{E}u^2\right)\end{pmatrix} \quad (1)$$

where λ_f and μ_f are two constants and $E = E_r/E_\infty$ is a dimensionless energy, E_r is the actual energy and $E_\infty = \hbar^2/2ma^2$.

The constants λ_f and μ_f are defined for the quantum ring by the boundary conditions: $F(1, C, E, m) = 0$ [18] and $F(u_e, C, E, m) = 0$ (figure 1). The same analytical form is obtained for the $g(v)$ function with the change $C \to -C$: $g(v) = F(v, -C, E, m)$. If $u_e = 0$ (quantum disc case), $\mu_f = 0$ [18]. If $C = 0$, the solutions of the problem contain simple $J_{m/2}(z)$ and $K_{m/2}(z)$ Bessel functions of complex variable z [13, 18]. This is in particular the case for the $m = 0$ ground state. The solutions with $C \neq 0$ are twice degenerate [18]. An equivalent description can be used for the parabolic cylindrical set of unit-less coordinates (u, v, z). The wavefunction appears as a product of functions of independent variables $\Xi(u, v, z) = f(u)g(v)h(z)$ for the quantum wire. The f and g functions [13, 14] contain two confluent hypergeometric functions of the first kind (figure 2).

The reduced energy E of the 1S ground state and the first excited 1P state may be calculated for the quantum ring with a flat base as a function of the reduced area S (figure 2). The energy of the ground state of the quantum wire with a flat base is represented by a dotted line on the same figure. The dimensionless product E^*S is represented in figure 2 as a function of the reduced section S. In the limit of a perfect 1D system ($S \to 0, u_e \to 1$), the same

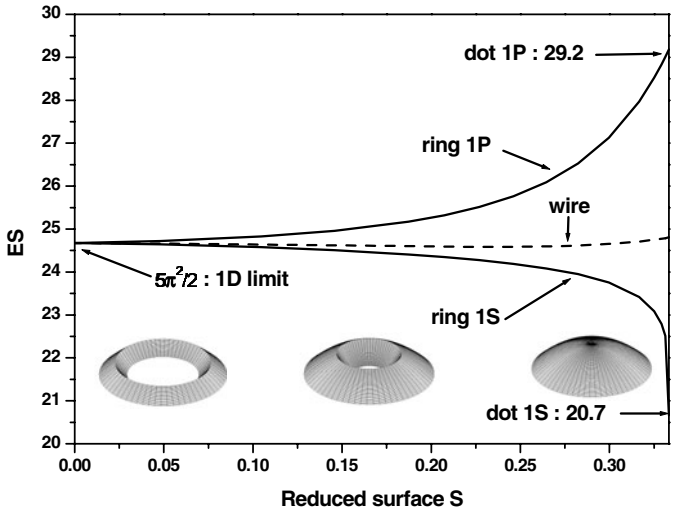

Figure 2. The dimensionless product E^*S, where $E = E_r/\frac{\hbar^2}{2ma^2}$ and $S = S_r/a^2$ is the reduced area of the cross-section, is represented as a function of the reduced section S, where a is the parameter of the parabolic metric. When $S \to 0$, the limit of a perfect 1D system is obtained for the 1S, 1P states of the quantum ring with a flat base and for the ground state of the cylindrical parabolic quantum wire (dotted line). In the limit $S \to 1/3$ for the quantum ring, the case of a 0D quantum dot is recovered. The product E^*S for the 1S state undergoes a very fast variation close to this limit. Schematic representations of the quantum ring geometries have been added.

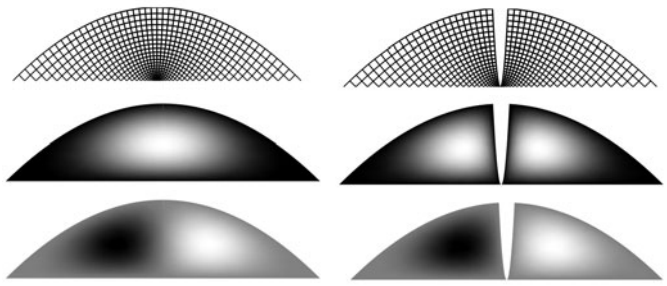

Figure 3. Cross section ((x, z) plane) of the parabolic mesh, the fundamental state 1S and the first excited 1P wavefunctions for a quantum lens (left-hand side) and a quantum ring with flat bases ($u_e = 0.05$, right-hand side).

value $E^*S = 5\pi^2/2 = 24.7$ is obtained in the three cases. In the limit of a 0D quantum dot ($S \to 1/3, u_e \to 0$) for the quantum ring, the eigenvalue for the 1S ground state is already known, $E^*S = 20.7$ [18]. The energy E of the 1S state undergoes, however, a very fast variation in the vicinity of this limit. In contrast, the variation of the energy E of the 1P state is smooth near the limit of the 0D quantum dot ($E^*S = 29.2$). It may be understood when considering that the 1S ground state of the 0D quantum dot has an electronic density maximum along the z-vertical axis [18]. It is then strongly modified when switching from a quantum dot geometry to a quantum ring geometry where the potential becomes infinite around the z-vertical axis. The 1S, 1P electronic wavefunctions for a dot ($u_e = 0$, on the left-hand side) and a ring ($u_e = 0.05$, on the right-hand side) with flat bases are represented in figure 3 together with the parabolic mesh. The modification of the wavefunction is continuous for the 1P state

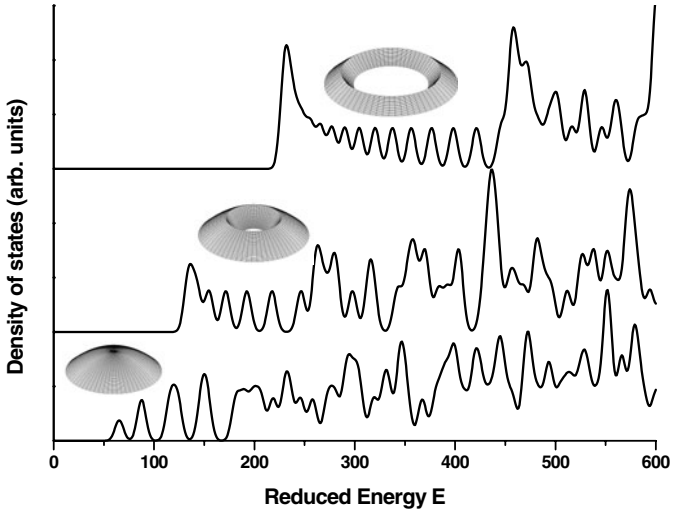

Figure 4. Representations of the electronic densities of states for a quantum lens (top) and two quantum rings with $u_e = 0.5$ (middle) and $u_e = 0.75$ (bottom). Schematic representations of the lens-like and volcano-like geometries have been added. The peaks have been convoluted by Gaussian functions with a full width at half maximum equal to 10 in reduced energy units.

because the electronic density distribution is very similar to both geometrical cases (figure 3). Experimental results for self-assembled InAs quantum rings grown on a GaAs substrate [5] indicate that the interband transition spectrum is different from that of self-assembled InAs quantum dots. In this work we confirm this observation, and we also precisely describe the electronic state variation when the geometry of the quantum object is continuously changed from a dot to a ring. Figure 4 represents a comparison between the electronic density of states of a quantum lens and two quantum rings with $u_e = 0.5$ and $u_e = 0.75$. The reduced energies of the two quantum wires have been calculated by considering that the volume is constant and equal to the volume of the quantum lens. It corresponds to a hypothesis that the ring formation from a dot mainly occurs through matter redistribution; this process has been observed experimentally [4, 6]. In addition, the peaks have been convoluted by Gaussian functions in order to take into account the experimental broadening effect. The full width at half maximum of these functions is equal to 10 in reduced energy units. The electronic density of states of the quantum ring showed at the top of the figure presents the behaviour of quasi-1D systems, whereas the density of the quantum lens (bottom of the figure) presents Gaussian-like features of quasi-0D systems.

The problem of electronic energy levels and wavefunctions in quantum dots and quantum rings was studied. Exact solutions for the symmetric and asymmetric quantum rings are found in a parabolic coordinate system. The continuous evolution from a 0D quantum dot to a perfect 1D quantum ring can be precisely described. A sharp variation of electronic properties appears at the early stage of the quantum ring formation for totally symmetric states of the quantum dot. The reason is the immediate build-up of a potential energy barrier at the centre of the ring structure. The study of the electronic density of states as a function of the quantum ring shape transformation indicates also a progressive change of dimensionality. Further work will focus on the study of various physical effects such as Stark shifts [18], many-body effects and Aharonov–Bohm magnetic shifts [6] which may be simplified by using simple analytical solutions. The method described in this letter also shows for the first time that not only simple

geometries but also complex geometries may be studied with orthogonal coordinates by using symmetry properties and special boundary conditions.

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