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Analytical solution of the Schrödinger equation for an electron confined in a triangle-shaped quantum well

Peter N. Gorley[a], Yuri V. Vorobiev[b,*], Jesús González-Hernández[b], Paul P. Horley[a,b]

[a]*Department of Physical Electronics and Non-Traditional Energy Sources, Chernivtsi National University, 2 Kotsyubynsky Str., 58012 Chernivtsi, Ukraine*

[b]*CINVESTAV-Querétaro, Libramiento Norponiente 2000, Fracc. Real de Juriquilla, 76230 Querétaro, Mexico*

Abstract

For the triangular-shaped quantum well, the electron wave functions and energy values are found by analytical solution of the Shrödinger equation. In approximation of impenetrable walls, two sets of solutions are obtained, one corresponding to the symmetric, and the other to antisymmetric wave functions. The distributions of the probability density give a clear picture of standing waves in a triangular-shaped plate. The comparison of the system energy levels with those obtained for quasi-periodic boundary conditions give reasonable coincidence. The results obtained proved to be useful in explanation of electronic optical absorption spectra of some of the organic colorants, on the basis of FEMO approach (free electron molecular orbitals); it could be used for other nanosystems with particles of triangular shape.

Keywords: Quantum well; Energy; Wave function; Absorption spectrum

1. Introduction

The approximation of a particle in a two-dimensional quantum well became very popular in the last two decades due to active investigation of the artificial quantum-confined systems (see, for example, Refs. [1–5]); besides, it is widely used for explanation of optical properties of the organic molecules on the basis of the FEMO approach (free electron molecular orbitals), treating an electron delocalized within a molecule [6–10]. Normally, the rectangular-shaped or circular well models are applied in the cases mentioned. However, in some cases, the triangular-shaped quantum well could be the better approximation: some of the organic dye molecules such as FD&C red No. 3 (erythrosin, shown in Fig.

*Corresponding author. Tel.: +52-442-211-9900; fax: +52-442-211-9939.
E-mail addresses: peter_gorley@altavista.com (P.N. Gorley), vorobiev@arcos.qro.cinvestav.mx (Y.V. Vorobiev).

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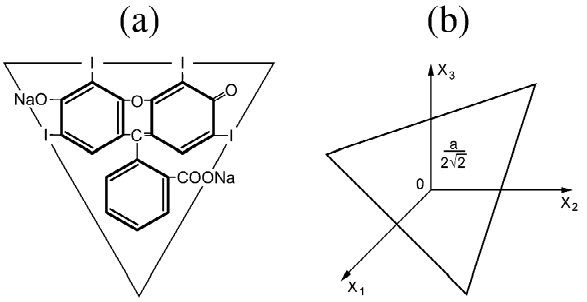

Fig. 1. The molecule of organic dye FD&C red No. 3 (a); the triangle used for theoretical considerations (b).

1) or Rhodamine have approximately triangular shape; this model also could be of interest in studying pyramid-shaped quantum confined systems easily obtained by etching of semiconductor surfaces, etc. Here we attempted the direct quantum mechanical treatment of the problem assuming impenetrable boundaries; the results obtained are compared with similar results for other types of two-dimensional wells and other boundary conditions.

2. Theory

We consider the electron delocalized in a triangular-shaped quantum well with infinitely high potential walls. To substantiate the example shown in Fig. 1, we must mention that in FEMO treatment of the organic molecules as two-dimensional quantum wells, it is usually accepted [6–8] that the walls of the well are situated at a distance of approximately one bond length from the boundary atoms of a molecule. Taking account of this, we have drawn the external triangle in Fig. 1a, considering it as the area of localization of an electron in FEMO approximation.

Taking the triangle to be equal-sided with the length of the side a we assume it to be placed into a right-hand cartesian reference system with axis x_1, x_2 and x_3 in the manner where the sides of the triangle are perpendicular to the axis (Fig. 1b). Then the equation of plane of the triangle could be written as:

$$x_1 + x_2 + x_3 = a/2\sqrt{2}, \tag{1}$$

where x_1, x_2 and x_3 are the coordinates of the points that belong to triangle.

Under assumptions made, the Schrödinger equation for the quantum particle is

$$-\frac{\hbar^2}{2m_0}\sum_{n=1}^{3}\frac{\partial^2\Psi}{\partial x_n^2} = E\Psi, \tag{2}$$

with wave function Ψ, energy E, and mass of the particle m_0. Introducing

$$k^2 = \frac{2m_0E}{\hbar^2}, \tag{3}$$

one can rewrite (2) as

$$\sum_{n=1}^{3} \frac{\partial^2 \Psi}{\partial x_n^2} + k^2 \Psi = 0. \tag{4}$$

As in this case the potential energy of the particle interaction is equal to zero, and the system of coordinates is cartesian, one can use method of variable separation, thus presenting Ψ as the products of three functions (Ψ_n), each one of its own variable.

This gives a general solution in a form

$$\Psi_n = A_n \exp(ik_n x_n) + B_n \exp(-ik_n x_n), \tag{5}$$

with additional condition

$$\sum_{n=1}^{3} k_n^2 = k^2. \tag{6}$$

Here A_n and B_n are integration constants, and i is imaginary unit. Transforming (5) to trigonometric functions, we get

$$\Psi = \prod_{n=1}^{3} [(A_n + B_n)\cos k_n x_n + i(A_n - B_n)\sin k_n x_n]. \tag{7}$$

To determine the exact wave function we need to imply the symmetry and boundary conditions, namely:

(1) *Symmetry condition*. As (5) does not change with inversion of coordinates $x_n \to -x_n$, it means that eigenfunctions of Hamiltonian should be even

$$\Psi_e(x_n) = \Psi_e(-x_n), \tag{8}$$

or odd

$$\Psi_o(x_n) = -\Psi_o(-x_n). \tag{9}$$

Therefore one needs to consider either even or odd wave functions; it is easy to show that condition (8) could be fulfilled for all the x_n in (7) when $A_n = B_n$, thus

$$\Psi_e = 8 \prod_{n=1}^{3} A_n \cos k_n x_{n,} \tag{10}$$

while (9) is valid when $A_n = -B_n$, that gives us

$$\Psi_o = -8i \prod_{n=1}^{3} A_n \sin k_n x_{n.} \tag{11}$$

(2) *Impenetrable potential barrier conditions*. As the particle cannot cross the borders, that implies that wave function has to be zero at the boundaries

$$\Psi_{e,o}(x_n = \frac{a}{2\sqrt{2}}, x_p, x_r) = 0 \quad (n,p,r = 1,2,3), \tag{12}$$

that leads to the discrete values of k_n, namely

(a) for the even wave function

$$k_{n_e} = (2m_{n_e} + 1)\frac{\sqrt{2}\pi}{a} \quad (m_{n_e} = 0,1,2,3,\ldots), \tag{13}$$

(b) for the odd wave function

$$k_{n_o} = 2\sqrt{2}\frac{\pi}{a}m_{n_o} \quad (m_{n_o} = 1,2,3,\ldots). \tag{14}$$

Here it is necessary to stress that when $m_{n_o} = 0$, the wave function Ψ_o, due to (11) turns to zero, thus the quantum particle cannot be in this quantum state, meaning that case $m_{n_o} = 0$ should be omitted from (14). Introducing (13) into (10) and (14) into (11), we obtain the expressions for the wave function of the particle:

(a) even case

$$\Psi_e = 8A_1A_2A_3\prod_{n=1}^{3}\cos k_{n_e}x_n, \tag{15}$$

(b) odd case

$$\Psi_o = -8iA_1A_2A_3\prod_{n=1}^{3}\sin k_{n_o}x_n \tag{16}$$

To find the value $A_1A_2A_3$ we use the wave function normalization

$$\int\int_S \Psi\cdot\Psi^* \mathrm{d}S = 1, \tag{17}$$

where S is the area of the triangle.

Having performed the necessary calculations, we obtain the expressions for wave functions and for the squared wave functions, that have the meaning of probability:

(a) even case

$$\Psi_e^2(x_1,x_2,x_3) = \frac{512}{3\sqrt{3}a^2}\cdot\frac{\prod_{n=1}^{3}\cos^2(2m_{n_e}+1)\sqrt{2}\pi\frac{x_n}{a}}{1+\frac{4}{\pi^2}\cdot\frac{4}{(2m_{n_e}+1)^2}}, \quad (m_{1_e} = m_{2_e} = m_{3_e} \equiv m_e), \tag{18a}$$

$$\Psi_e^2(x_1,x_2,x_3) = \frac{128}{\sqrt{3}a^2}\cdot\frac{\prod_{n=1}^{3}\cos^2(2m_{n_e}+1)\sqrt{2}\pi\frac{x_n}{a}}{1+\frac{4}{\pi^2}\cdot\sum_{n=1}^{3}\frac{1}{(2m_{n_e}+1)^2}}, \quad (m_{1_e} \neq m_{2_e} \neq m_{3_e}, \text{ or } m_{n_e} = m_{p_e} \neq m_{r_e}; (n,p,r = 1,2,3)) \tag{18b}$$

(b) odd case

$$\Psi_{o}^{2}(x_1,x_2,x_3) = \frac{512}{3\sqrt{3}a^2} \cdot \prod_{n=1}^{3} \sin^2 2m_{n_o} \sqrt{2}\pi \frac{x_n}{a}, \quad (m_{1_o} = m_{2_o} = m_{3_o} \equiv m_o) \tag{19a}$$

$$\Psi_{o}^{2}(x_1,x_2,x_3) = \frac{128}{\sqrt{3}a^2} \cdot \prod_{n=1}^{3} \sin^2 2m_{n_o} \sqrt{2}\pi \frac{x_n}{a}, \quad (m_{1_o} \neq m_{2_o} \neq m_{3_o}, m_{n_o} = m_{p_o} \neq m_{r_o}; (n,p,r = 1,2,3)) \tag{19b}$$

Since we applied to the general solution (7) the symmetry conditions (8) and (9) and the boundary condition (12), the expressions (18) and (19) obtained here represent the unique solution of the problem.

It follows from (18 and 19) that the probability for the particle to exist in the most symmetric states for both even and odd states (18a) and (19a) is greater than for the other states.

Energy values for the particle in the system considered could be found by introducing (13) and (14) into (6) and taking into account (3):

(a) for even states

$$E_e = E_0 \cdot \sum_{n=1}^{3} (2m_{n_e} + 1)^2, \tag{20}$$

(b) for odd states

$$E_o = 4E_0 \cdot \sum_{n=1}^{3} m_{n_o}^2, \tag{21}$$

where

$$E_0 = \frac{\hbar^2 \pi^2}{m_o a^2}. \tag{22}$$

From (20) and (21) it follows that quantum states of the particle are characterized by the discrete values of energy. Even and odd wave functions in this respect go one after another, and the smallest value of energy corresponds to the even state. It also seen that the same value of energy could correspond to different combinations of quantum numbers, hence giving us degenerated energy levels. For example:

(a) for even states $E(1,1,1) = E(2,0,0) = 27E_o$.

(b) for odd states $E(3,3,3) = E(5,1,1) = 108E_o$.

3. Comparison with traditional two-dimensional problems

In many cases, the rectangular well is a good approximation for FEMO analysis (for example, in description of the properties of organic colorants like Fast Green or Basic Yellow, see Refs. [9,10]). For this well with dimensions L_1, L_2 the analytical solution of the Shrödinger equation again has the

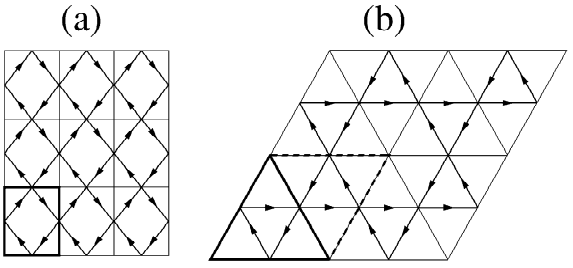

Fig. 2. Laboratory system geometry.

form (5) with two variables, there are also odd and even functions, and the electron energy levels for the case of unpenetrable walls are given by the expression

$$E = (h^2/8m_o)\,(n^2/L_1^2 + m^2/L_2^2), \tag{23}$$

n and m being the quantum numbers, even for the even solutions and odd for the odd ones.

It is interesting to note that the same energy spectra for the particle in the rectangular well could be obtained using the quasi-periodic boundary conditions, considering the potential 'walls' of the well like mirrors, which makes a quasi-periodic structure from the one cell, as is shown in Fig. 2a (here the arrows show the directions of a particle's motion, i.e., the **k**-vector, and the corresponding reflections). It is evident, that the cell with its reflections form the periodic structure with the period doubled compared to the cell dimensions. Applying to this structure the Born–von Karman boundary conditions, we again get expression (23) for the energy.

A similar consideration based on the particle reflections by the walls of the well, could be applied to the triangular-shaped well (Fig. 2b). We see, again, that the periodic structure is formed, and the translation symmetry corresponds to the translations of the rhombus consisting of the two cells in the directions of its sides. Using the Born–von Karman boundary conditions, we obtain for the energy levels

$$E = (2\,h^2/3m_o a^2)(n^2 \pm n\,m + m^2) \tag{24}$$

This expression, although different from the ones obtained earlier ((20)–(22)), describes a rather similar energy spectrum. Fig. 3a shows the first five energy levels given by (20)–(22), whereas Fig. 3b shows those given by (24). A close resemblance of the two spectra could be seen (we made the corresponding comparison up to 15 levels, with similar result).

Fig. 4 shows distributions of probability density for different states of the particle in rectangular and triangular wells. In all cases the pictures obtained show the definite pattern of standing waves in a corresponding two-dimensional system, formed by reflections of the de-Broglie waves by the well's

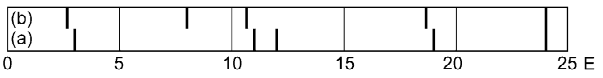

Fig. 3. Energy spectra given by(a) (20)–(22); (b) (24).

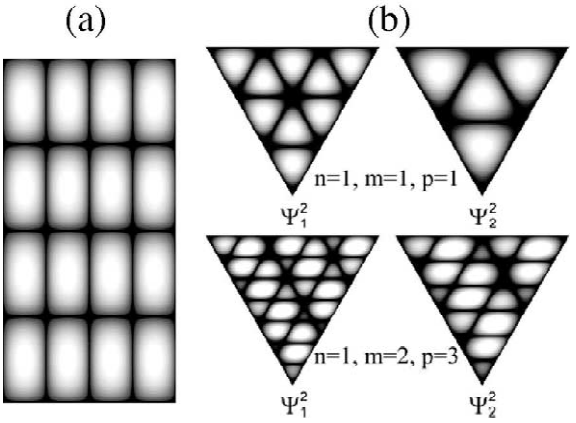

Fig. 4. Probability density of wavefunctions for (a) rectangular quantum well with $n = m = 4$, (b) triangular quantum wells with given quantum number values.

wall. We conclude that this result substantiates the idea of the mirror-like walls and the use of quasi-periodic boundary conditions.

Calculations, performed with experimental data for energy spectra of the different organic dyes (to be published separately) show the applicability of the approach developed. The proposed methodology to calculate the wave functions in triangular-shaped quantum well could be applied to other cases with triangular geometry.

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References

[1] G.D. Sanders, Y.C. Chang, Theory of photoabsorption in modilation-doped semiconductor quantum wells, Phys. Rev. B 35 (1987) 1300–1315.
[2] D.A. Kleinman, Binding energy of electron-hole liquid in quantum wells, Phys. Rev. B 33 (1986) 2540–2549.
[3] A.E. Ruckenstein, S. Schmitt-Rink, R.C. Miller, Infrared and polarization anomalies in the optical spectra of modulation-doped semiconductor quantum well structures, Phys. Rev. Lett. 56 (1986) 504–507.
[4] J. Marzin, J. Gérard, Experimental probing of quantum-well eigenstates, Phys. Rev. Lett. 62 (1989) 2172.
[5] G.A. Baraff, Semiclassical description of electron transport in semiconductor quantum-well devices, Phys. Rev. B 55 (1997) 10745.
[6] J.R. Platt, The box model and electron densities in conjugated system, J. Chem. Phys. 22 (1954) 1448–1455.
[7] J. Griffits, in: Colour and Constitution of Organic Molecules, Academic Press, London, 1976.
[8] J.B. Birks, in: Photophysics of Aromatic Molecules, Wiley-Interscience, London, New York, Sidney, Toronto, 1970.
[9] J.J. Pérez-Bueno, L.L. Díaz-Flores, F.J. Espinoza-Beltrán et al., Energy spectra of dyes embedded in SiO_2 sol–gel glass, Rev. Mex. Fís. 46 (2000) 67–71.
[10] J.J. Pérez-Bueno, L.L. Díaz-Flores, J.F. Pérez-Robles et al., Optical processes in SiO_2 sol–gel glass colored with organic dyes, Inorg. Mater. 36 (2000) 1258–1266.