Approaching to nanostructures using basic concepts of quantum mechanics

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In this work we discuss some concepts of quantum mechanics showing the result for the ground state energy of the infinite potential well that, together with elementary thermal physics concepts applied to semiconductors, help us to estimate the size of nanostructures. The energy value of the infinite potential well is compared with the finite potential well, some results were obtained with numerical calculations using basic quantum mechanics, particularly we used the BenDaniel-Duke model used for semiconductor junctions to analyze the structure GaAs-$Al_{1-x}Ga_xAs$, the energy levels were obtained of the confined states in the quantum well of the nanostructure in function of Al percentage. This system is representative of nanostructures quantum devices, currently under study in electronic solid state physics. This presentation could be very useful to teach in undergraduate applied physics courses.

Keywords: Applied modern physics; potential wells; nanostructure devices.

En este trabajo discutimos algunos conceptos de mecánica cuántica mostrando el resultado para la energía de estado base del pozo de potencial infinito que conjuntamente con conceptos elementales de física térmica aplicados a semiconductores nos son útiles para estimar el tamaño de nanoestructuras. El valor de la energía del pozo de potencial infinito es comparado con el pozo de potencial finito, algunos resultados fueron obtenidos con cálculos numéricos usando mecánica cuántica básica, particularmente usamos el modelo de BenDaniel-Duke para analizar la estructura de GaAs-$Al_{1-x}Ga_xAs$, se obtienen los niveles de energía de los estados confinados en el pozo cuántico de la nanoestructura en función del porcentaje de Al. Este sistema es representativo de dispositivos cuánticos nanoestructurados estudiados actualmente en la física electrónica del estado sólido. Esta presentación puede ser útil para enseñanza a nivel licenciatura o posgrado en cursos de física aplicada.

Descriptores: Física moderna aplicada; pozos de potencial; dispositivos nanoestructurados.

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1. Introduction

From our experience communicating the basic principles of Quantum Mechanics to the students, we found that the concepts are very well understood, since we depart from the classical model of the hydrogen atom, describing the movement of the electron around the proton as particles and using the conservation of energy principle. Then, we show the wave equivalence of the electron, taking into account the equivalency of the perimeter of his orbit with the wavelength that represents it according to De Broglie, and the conservation of energy principle, that it is implicit in the Schrödinger's Equation. This is a new concept to the students, in which they may be confused at the beginning, because the electron that was at first considered a particle now shows the behavior of a wave [1].

When the movements of the electrons in a material are restricted to a very small region, we say that they are confined, and when the size of such region is equivalent to the De Broigle wave length, we see behaviors that can't be explained through the classical concepts. Such behaviors appear when the size is given in nanometric dimensions and can be explained only from a quantum mechanics point of view.

We calculated the energy levels for an electron trapped in an infinite potential well and showed that the width of the well is of a nanometric size. This finally allows us to adapt this focus to the concepts of Nanotechnology, and in the possibilities of new materials with physical innovative properties and practical applications as, for example, the semiconductors. This focus is useful to approach the scientific knowledge in the matter to students that do not have a strong educational background in physics.

The approach presented here, give the quantum mechanics result for an infinite potential well, which allows handling the calculation of a nanostructure if it is used as a starting point. This is valuable in the classroom to introduce, for the first time, simple quantum mechanics results and its use for application in nanostructures. Formal exact results of complex quantum systems can be found in the literature [2].

2. Theory and calculations

The ground state energy of the potential well, with width L is:

$$E = \frac{h^2}{8mL^2} \tag{1}$$

The value of the Eq. (1) corresponds to the ground state of an infinite potential well [3].

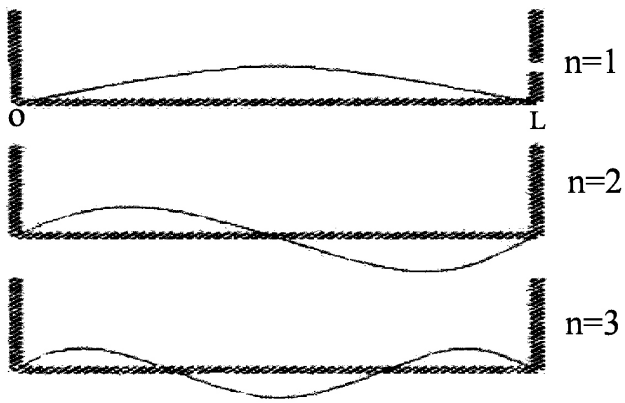


FIGURE 1. The first three quantum states of a quantum well.

The consideration of infinite well barrier means physically that the trapped particle has energy much smaller than the size of the well barrier.

To apply the results to an electron in a system with quantum size effects for considering it moving in a nanostructure confining in a region L [4]. In particular, in semiconductor materials we observe this quantum confinement by its optical properties.

We can consider the dimension of that system for an electron moving at temperature T with the use of an elementary concept of thermal physics *i.e.* the equipartition principle of energy. The electron is moving only in one direction, using this principle the result is of the order of (1/2)kT, where k is the Boltzman constant [5] then, with the help of Eq. (1), L is:

$$L = \frac{1}{2}\frac{h}{\sqrt{mkT}} \tag{2}$$

It is generally accepted that the calculation of static energy levels within quantum wells should take account for the variation in the effective mass m^* [6]. The electron is moving with an equivalent mass m* in the semiconductor [7], such statement is rigorously demonstrated in solid state textbooks [8], a typical value is $m^* = 0.1m_o$. At room temperature kT=0.025 electron Volts (eV). Then we find that we must have L in the order of 10 nanometers, this is the origin of the nanostructure word, that is no more than: a structure measured in nanometers. Thus a "thin semiconductor layer" of thickness of 1 micrometer does not has a size for confinement effects. It is in fact a crystal which would not exhibit any quantum size effects. To observe quantum size effects we require thinner layers. The minimum state of a 10 nm GaAs quantum wells for the infinite well has a value of 57 meV [9], a value accordingly with the experiment is of the order of 32 meV obtained with a finite potential well. We can calculate this result using formal quantum mechanics methods [3].

In this problem, the infinite well model overestimates the confinement energies, but is useful for the discussion of the physics because of its simplicity. For more exact values you can see the literature [10], but here we give a short discussion of the important facts about the quantum confinement.

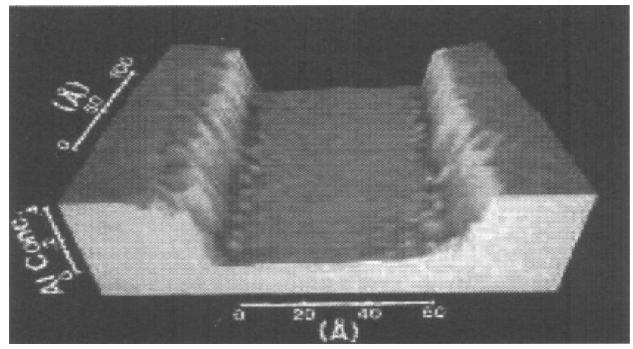


FIGURE 2. A micrograph of a heterostructure, gratuitous, obtained form the web.

3. Quantum wells

For the potential well, quantum mechanics establishes that an electron cannot be found in any state of energy, the boundary conditions implies that wave is equal to zero in the walls of the potential well, being the most energetic states those having more nodes (n) in the inside of a quantum well (Fig. 1). At the present and thanks to the technological advances it is possible to manufacture physical systems where they can confine electrons in nanoscale structures and if the system has two dimensions we have the quantum wells.

In a quantum well the electrons are confined in one direction only (vg. the z direction), while in the plane (x,y) they move freely. At the direction z the electronic states are discreet, on the other hand in (x,y) the possible states are continuous.

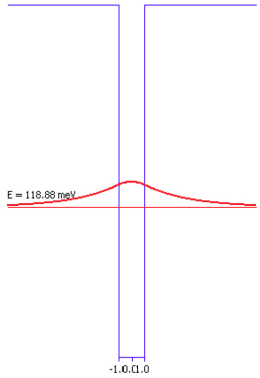
The present-day technique of epitaxial growth for molecular beams, allows joining two different materials to make a flat heterostructure between two semiconductors. A quantum well can be obtained when a plate of a semiconductor is placed (for example GaAs) between two semiconductors of prohibited bigger interval itself ($Al_{1-x}Ga_xAs$) Fig. 2, [11].

4. Heterojunctions and heterostructures

The effective mass approximation it's used for a bulk crystal, meaning the crystal is very large with respect to the scale of an electron wave function which is effectively infinite. When two such materials are placed adjacent to each other they form a heterojunction. In such case the Schrödinger's equation would be used for any one band, taking the effective mass to be the same in each material. The heterostructures are formed from multiple heterojunctions.

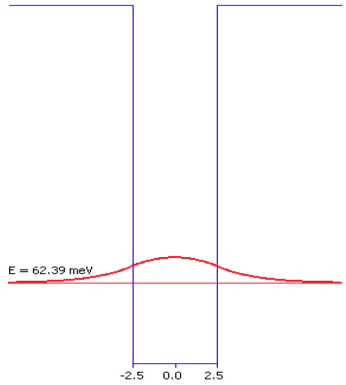
Starting from Schrödinger's equation a mathematical model that allows describing the electronic state of the heterostructure of (GaAs-$Al_{1-x}Ga_xAs$) is the one of BenDaniel-Duke used in semiconductor junctions [12]. Considering E_1 and E_2 as the energies of the borders of the bands in both semiconductors and $V_0 = E_2 - E_1$ tells how much are apart between the borders, then the equation that describes the system is the Schrödinger equation (3) when the transversal

GRAPH 1

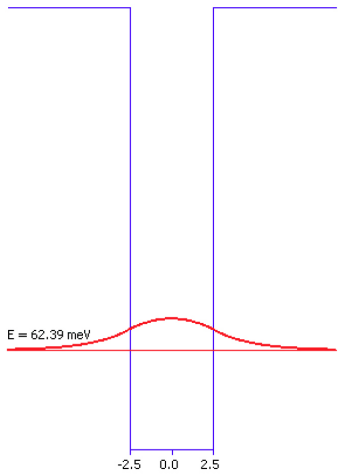


% Al =.2 α =2 nm

GRAPH 2

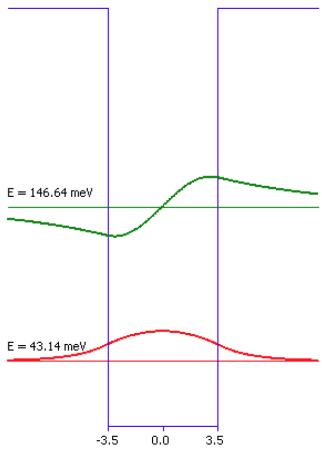


% Al = .3 α =5 nm

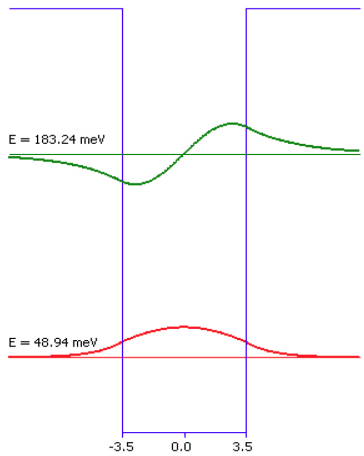


% Al =.2 α =5 nm

% Al =.3 α =5 nm



% Al =.2 α =7 nm



% Al =.3 α =7 nm

FIGURE 3. Calculations of the heterostructure with different aluminum concentrations.

moment in the plane (x,y) is equal to zero and the direction of growth z is perpendicular to the plane.

$$\left(-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m^*}\frac{d}{dz}+V(z)\right)\psi(z)=E\psi(z) \qquad (3)$$

The value of $V(z)$ is equal to zero at the plane of GaAs of thickness α while it takes the value V_0 in $Al_{1-x}Ga_xAs$. The condition of contour in $z=0$ can be obtained integrating the Eq. (3) in the neighborhood of that plane, then in order to avoid infinite kinetic energies it is seen that both

$$\psi(z) \quad \text{and} \quad \frac{1}{m^*}\frac{dx(z)}{dz} \qquad (4)$$

must be continuous.

The solutions of the equation for the involving function in a quantum well corresponds to the confined states which can be classify according to their parity.

Semiconductor quantum wells are examples of nanostructures built by artificial crystals in layers of different materials grown on top of a thicker crystal. The structures are made by the specialized epitaxial crystal growth techniques. The layer thickness of the crystal growth can be controlled with atomic precision. This makes it easy to achieve the thin layer thickness required to observe quantum confinement of the electrons in a semiconductor at room temperature. An example of a heterostructure nanostructure device is a series of single GaAs/AlGaAs quantum wells. The single quantum well is formed in the thin GaAs layer sandwiched between AlGaAs layers. Using the above theory we present the states of this system. The corresponding levels of energy are obtained by solving numerically the transcendent equations considering the small masses of the electron and the hole.

Even

$$\psi(z)=\begin{cases}\cos(k\alpha/2)\exp\left[\beta(z+\alpha/2)\right] & z<-\alpha/2\\ \cos(kz) & |z|\le\alpha/2\\ \cos(k\alpha/2)\exp\left[\beta(-z+\alpha/2)\right] & z>\alpha/2\end{cases}$$

Odd

$$\psi(z)=\begin{cases}\sin(k\alpha/2)\exp\left[\beta(z+\alpha/2)\right] & z<-\alpha/2\\ \sin(kz) & |z|\le\alpha/2\\ \sin(k\alpha/2)\exp\left[\beta(-z+\alpha/2)\right] & z>\alpha/2\end{cases}$$

Using these trial forms of the wave function in their corresponding Schrödinger's equations, we obtain:

$$K=\frac{\sqrt{2m*E}}{\hbar} \quad \beta=\frac{\sqrt{2m*(V-E)}}{\hbar} \qquad (5)$$

Solving numerically the transcendental equations we can get the corresponding energy levels.

Graphs 1 and 2 in Fig. 3 show the values of the energy of the status restricted in terms of the aluminum percentage and of the thickness of the cape of GaAs.

This type of structure is a multiple quantum wells. In this system the individuals are isolated from each other, and the properties are associated to the single quantum wells. They are often used in optical applications to give a usable optical density. It would be very difficult the optical absorption of a single 10 nm thick quantum well, simply because it has so little material to absorb the light.

5. Conclusions

The expression known of the infinite potential well, and the exact value of the ground state of energy are very useful to introduce an idea of modern systems handled in solid state physics. The use of simple arguments give to undergraduate students in intermediate courses of Applied Modern Physics in Engineering, Chemistry and Physics undergraduate and graduate Programs, the opportunity to obtain a primary knowledge of the nanostructure building and a first idea of this modern systems handled actually in applied physics.

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