The inverse problem in potential wells

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We study the solution of the inverse spectral problem of a potential well (PW). This problem constitutes a good exercise for the understanding of the Schrödinger equation, especially if we take into account that often this topic is not undertaken in regular courses of Quantum Mechanics. This exercise also propitiates the training of the students in the solution of this kind of problems, which frequently appears in research experimental work. We think that the exercises that are demonstrated in this paper could·be included in Quantum Mechanics regular courses. The inverse problem presented here consists in the reconstruction of a PW, *i.e.*, find the height of the barrier and the width of the well, provided the values of the discrete energy levels or the transition energies between them are known. We show three different cases of this problem referred to rectangular PWs. In all cases, the equations are deduced and the developed method is illustrated graphically.

Keywords: Electron states in quantum wells

En el presente trabajo se estudia la solución del problema inverso espectral de un pozo potencial (PP). Este problema es un buen ejercicio para la comprensión de la ecuación de Schrödinger, sobre todo si se tiene en cuenta que por lo general no es abordado en los cursos regulares de mecánica cuántica. Asimismo, este ejercicio propicia el entrenamiento de los estudiantes en este tipo de problemas, que aparecen con frecuencia en la investigación experimental. Nosotros somos de la idea que los ejercicios que se desarrollan en este trabajo podrían ser incluidos en los cursos regulares de mecánica cuántica. El problema inverso consiste en hallar la forma de un PP, o sea encontrar la altura de la barrera y el ancho del pozo, partiendo del conocimiento de los valores de los niveles discretos de energía o los valores de las energías de las transiciones entre estos niveles. Se estudian tres casos diferentes de este problema aplicado a los PP rectangulares. En todos los casos estudiados se deducen las ecuaciones y el método seguido se ilustra graficamente con ejemplos concretos.

Descriptores: Estados electrónicos en pozos cuánticos

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1. Introduction

The study of potential wells (PWs) is an essential topic in the undergraduate course of quantum mechanics, and it constitutes an indispensable exercise to understand the Schrödinger equation related to the stationary states of the particle motion. Although this is an idealized problem, it permits the comprehension of the methods of quantum mechanics. This topic appears in all textbooks; see for example Refs. 1–4. The problems presented there are guided to obtain the discrete, confined energy spectrum (E_n) and the particle wave function (ψ_n), provided the potential well (V) is known $\{V \rightarrow E_n, \psi_n(x)\}$. This is refereed to as the direct problem. However, when performing experiments one observes the energy spectrum $\{E_n\}$ or the scattered particles by a PWs. The former situation appears, for example in layered semiconductor structures. The widely used type I heterostructure quantum well (QW) are formed with a narrow bandgap semiconductor sandwiched by a wider bandgap semiconductor. In this case, the band discontinuities are such that both band edges of the smaller gap material lie below those of the wide-bandgap material. As a result, we obtain two PWs, the conduction band PW and the valence band PW. Optical spectroscopy experiments on this semiconductor PWs manifest the electron-photon interaction, which leads to transitions of electrons between the discrete energy levels of the two wells accompanied by the absorption or emission of photons [5–8]. Another example is the "photonic potential well" or dielectric waveguide. This is a structure where the photons are confined in a dielectric slab of higher refractive index sandwiched by lower refractive index materials, the profile of the whole structure forms the refractive index potential $n(x)$. Here, we measure the effective index of refraction $\{N_m\}$ of the waveguide modes which constitute the discrete confined levels [9].

Sometimes, it is required to restore the form of the well. This is referred to as the inverse spectral problem (ISP), *i.e.*, $\{E_n \rightarrow V(x)\}$, $\{N_m \rightarrow n(x)\}$ [9, 10].

The "inverse spectral problem" is not considered in regular courses of quantum mechanics although very often the experimental research work leads to it. For these reason we consider that the ISP must be included in regular courses of quantum mechanics, within the practice of the Schrödinger equation.

It is important to mention the inverse scattering problem (ISP) commonly treated, in regular courses of quantum mechanics. Here, the potential is obtained from the data of the amplitude (S) of the scattered particles by the potential, $\{S \to V\}$. We want to stress that these two inverse problems are very related to each other. The relation is so closed that Borg [11] demonstrated that in general, the knowledge of the single spectrum E_n is not sufficient to determine $V(x)$ [12]. This means, that in the traditional formulation of the inverse problem, for a purely discrete spectrum of bound states it is required to know two sets of parameters; besides the energy eigenvalues E_n, one must also know the normalization amplitudes of the wavefunction $\{c_n\}$ [13]. However, for symmetric potentials $V(x) = V(-x)$ the knowledge of E_n is sufficient and no additional data is required [12, 14]. Based on this statement the authors in Ref. 15 have developed and tested an algebraic technique for one-dimensional reflectionless PWs. It was found that the reconstruction of an infinite parabolic PW becomes better with increasing number of bound states N. On the other hand, the reconstruction of an infinite rectangular PW turned out to be significantly worse than for the parabolic and linear ones. Using the formalisms of Kay and Moses [16] and that of Thacker *et al.* [15], P. Asthana and A.N. Kamal [17] have studied the approximate reconstruction of different types of symmetric reflectionless PWs from their bound-state energies. They found that even if the reflection coefficient is not identically zero but a rapidly diminishing function of the particle wavenumber k, the procedure will lead to a reconstructed potential which will be reasonably close to the actual potential. The finite rectangular and the secant square PWs have reflection coefficients decaying extremely slowly with k and hence, the agreement between the actual potential and the reflectionless reconstruction is poor.

Another nice and interesting treatment of the ISP is reported in Ref. 10 for the case, when the potential $V(x)$ is a gradual varying function for which the semi-classical WKB approximation can be applied. In that work the author shows the inversion of the WKB formula for the Bohr-Sommerfeld quantisation rule to determine $V(x)$. Unfortunately, this approach has exact analytical solution for a very reduce class of PWs. Obviously, this technique can not be applied to rectangular PWs.

As we can see, there is not a suitable formalism for the reconstruction of rectangular PWs. However, in the field of semiconductor and photonic PWs the techniques of preparation of these systems are very sophisticated and the QW/barrier interface are very abrupt. The extension of the interface can be less than the lattice parameters or few of them. Thus, one can treat these abrupt heterostructures as rectangular PWs whose thickness and the barrier height are not known. This fact leads to a tremendous simplification of the problem. Indeed, as will be demonstrated bellow, the $\{E_n \to V\}$ problem in this case is reduced to the solution of a system of transcendental equations.

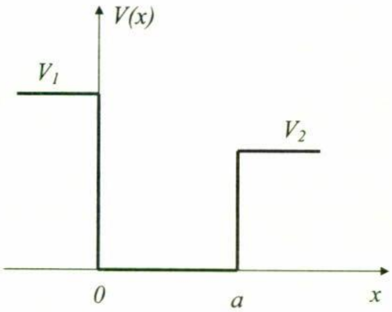

FIGURE 1. Scheme of an asymmetric potential well.

This paper discusses a method to find the shape of a rectangular PW; $V(x)$ using the energy spectrum $\{E_n\}$ as the input. The approach differs from the traditional direct problem method, where we seek for the values of the discrete energy levels varying the parameters of the PW, *i.e.*, the width and the barrier height, until one finds a well whose discrete energy levels match with the experimentally measured.

We present the solution of the ISP for three different situations. In the first two exercises, we reconstruct a symmetric and an asymmetric PWs. The third exercise is the reconstruction of a symmetric PWs starting from the transition energies between the discrete levels. In all cases, we illustrate the method with a particular example.

2. Theory

We begin with a conventional problem in quantum mechanics, namely to find the energy levels and the wave function of a particle in an asymmetric PW (see Fig. 1) and investigate the case $V_1 = V_2$ [1]. The dispersion law of the discrete energy levels in the well is given by

$$\frac{a\sqrt{2\mu E_n}}{\hbar} = n\pi - \arcsin\sqrt{\frac{E_n}{V_1}} - \arcsin\sqrt{\frac{E_n}{V_2}}, \qquad (1)$$

where a and V_1, V_2 stand for the thickness and the barrier heights of the PW respectively, E_n is the energy of the n discrete level, n is the quantum number of the level, μ denotes the mass of the particle, and $\hbar\,(\hbar = h/2\pi)$ is the Planck's constant.

2.1. Symmetric potential well

First, we show the method in the simplest case of a symmetric potential well, ($V_1 = V_2 = V$). For a symmetric PW, it is enough to know the energy of two levels. Let us consider that we have "measured" the first and the second levels, denoted by E_1 and E_2 , respectively, then from (1) one gets

$$a = \frac{\hbar}{\sqrt{2\mu E_1}}\left(\pi - 2\arcsin\sqrt{\frac{E_1}{V}}\right). \qquad (2)$$

This equation defines the width a as a function of the barrier height V, given the energy of the first level E_1 as a parameter, in other words $a = f_{E_1}(V)$. Thus, all the wells with widths a and barrier heights V that verify the relation (2) will have the first energy level equal to E_1.

In a similar way, the dependence of the width a on the barrier height V of all the wells that have the second energy level equal to E_2 is

$$a = \frac{\hbar}{\sqrt{2\mu E_1}}\left(2\pi - 2\arcsin\sqrt{\frac{E_2}{V}}\right) \tag{3}$$

This functional dependence has the form $a = f_{E_1}(V)$, where E_2 is a parameter. It is evident that for the PW with the two first level equals to E_1 and E_2, the equation

$$f_{E_1}(V) = f_{E_2}(V) \tag{4}$$

for the barrier height V is satisfied. Let us denote the root of this transcendental equation by $V_{\rm sol}$. The solution of the ISP is completed when the width of the PW is calculated; it is obtained from $a_{\rm sol} = f_{E_1}(V_{\rm sol})$ or $a_{\rm sol} = f_{E_2}(V_{\rm sol})$.

Next, we illustrate the method with the following example: Suppose it is given an hypothetical PW with $a = 15$ nm, $V = 0.31$ eV and $\mu = 0.0665\, m_0$ (m_0 denotes the mass of the free electron). This is the conduction band PW at the Γ point of a $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ ($x = 0.345$) heterostructure. Such a PW contains four energy levels with energies: $E_1 = 0.01796$ eV, $E_2 = 0.071105$ eV, $E_3 = 0.15665$ eV and $E_4 = 0.26517$ eV. Suppose that we only know the values of the first two energy levels E_1 and E_2. Figure 2 shows the dependencies of the width a on the barrier height V for all the PWs containing $E_1 = 0.01796$ eV and $E_2 = 0.071105$ eV. The crossover point of these curves, corresponds to the well that has the energy levels $E_1 = 0.01796$ eV and $E_2 = 0.071105$ eV simultaneously. The abscissa of this point is the root $V_{\rm sol} = 0.31$ eV of the transcendental equation $f_{E_1}(V) = f_{E_2}(V)$, and its ordinate $a_{\rm sol} = 15$ nm is determined by $a_{\rm sol} = f_{E_1}(V)$ or $a_{\rm sol} = f_{E_2}(V)$. See that the well has been reconstructed exactly.

2.2. Asymmetric potential well

Now, we consider an asymmetric rectangular PW. This situation is more complicated than the previous one, but the idea for the solution remains the same; it consists in expressing the width a of the well as a function of the barrier heights V_1 and V_2, taking the discrete energy levels as parameters. The problem has three unknown variables (V_1, V_2 and the well width, a), so we need to know three discrete energy levels.

If we substitute the values of the first three discrete energy levels E_n, where $n = 1$, 2 or 3 in Eq. (1) the width of the well as a function of the barrier heights can be written as:

$$a = \frac{\hbar}{\sqrt{2\mu E_n}}\left(n\pi - \arcsin\sqrt{\frac{E_n}{V_1}} - \arcsin\sqrt{\frac{E_n}{V_2}}\right). \tag{5}$$

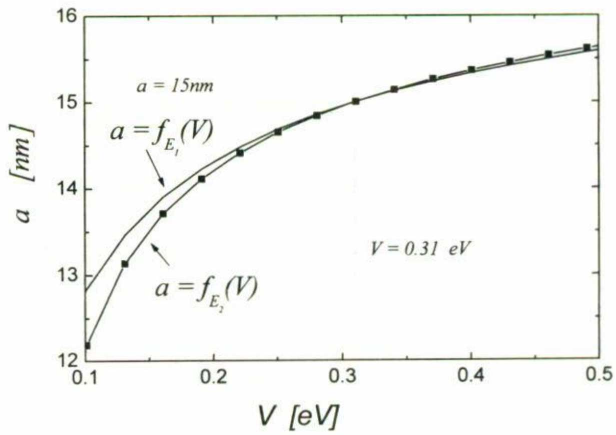

FIGURE 2. Graphic solution of Eq. (4). The curves $f_{E_1}(V)$ and $f_{E_2}(V)$ represent all the wells with energies E_1 and E_2 respectively. The intersection point $f_{E_1} = f_{E_2}(V)$ corresponds to a well with the barrier height $V = 0.35$ eV and width $a = 15$ nm.

We can eliminate the width a in Eqs. (5) and get the following system of equations:

$$\frac{2\pi - \arcsin\sqrt{\frac{E_2}{V_1}} - \arcsin\sqrt{\frac{E_2}{V_2}}}{\pi - \arcsin\sqrt{\frac{E_1}{V_1}} - \arcsin\sqrt{\frac{E_1}{V_2}}} = \sqrt{\frac{E_2}{E_1}}, \tag{5a}$$

$$\frac{3\pi - \arcsin\sqrt{\frac{E_3}{V_1}} - \arcsin\sqrt{\frac{E_3}{V_2}}}{\pi - \arcsin\sqrt{\frac{E_1}{V_1}} - \arcsin\sqrt{\frac{E_1}{V_2}}} = \sqrt{\frac{E_3}{E_1}}. \tag{5b}$$

Equation (5a) represents all the wells that have the first and second discrete energy levels equal to E_1 and E_2 respectively with the same well width. On the other hand, equation (5b) represents the same situation, but for the first and third discrete energy levels (E_1, E_3), *i.e.*, Eqs. (5a) and (5b) establish the dependencies for the barrier heights V_1 and V_2 of the wells that contain the levels E_1 and E_2, as well as E_1 and E_3, respectively. In other words, Eq. (5a) defines V_1 as an implicit function of V_2; *i.e.*, $V_1 = f_{E_1,E_2}(V_2)$ so that E_1 and E_2 are in the well. In a similar way, Eq. (5b) defines V_1 as an implicit function of V_2; $V_1 = f_{E_1,E_3}(V_2)$, so that E_1 and E_3 are in the well. The solution of the system (5a)–(5b) is reduced to the solution of the transcendental equation

$$f_{E_1,E_2}(V_2) = f_{E_1,E_3}(V_2). \tag{6}$$

Let the root of Eq. (6) be $V_2^{(\rm sol)}$, we complete the solution of the system evaluating the value $V_2^{(\rm sol)}$ in one of the functions $V_1 = f_{E_1,E_2}(V_2)$ or $V_1 = f_{E_1,E_3}(V_2)$; *i.e.*, $V_1^{\rm sol} = f_{E_1,E_2}(V_2^{\rm sol})$ or $V_1^{\rm sol} = f_{E_1,E_3}(V_2^{\rm sol})$.

The solution of the inverse problem is completed when we substitute the barrier heights $V_1^{\rm sol}$ and $V_2^{\rm sol}$ in one of the Eqs. (5) to find the well width $a_{\rm sol}$.

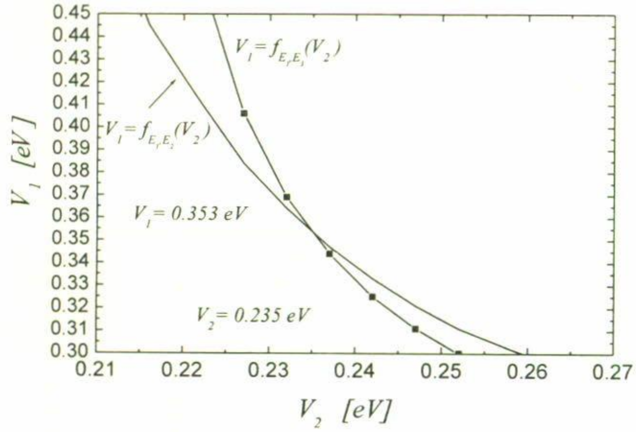

FIGURE 3. Graphic solution of Eq. (6). The intersection point $f_{E_1,E_2}(V_2) = f_{E_1,E_3}(V_2)$ gives the heights of the barriers V_1 and V_2. Knowing already V_1 and V_2 the well width is found from any of Eq. (5).

We illustrate the method with a particular example. Let us consider an asymmetric PW (see Fig. 1) with $a = 13.5$ nm, $V_1 = 0.353$ eV, $V_2 = 0.235$ eV and $\mu = 0.0665$ m$_0$. This PW has the following energy levels: $E_1 = 0.0211027$ eV, $E_2 = 0.0830912$ eV and $E_3 = 0.1799534$ eV.

Figure 3 illustrates the intersection of the curves which represents the dependence between V_2 and V_1 for all wells that have the same width and the energy levels ($E_1 = 0.0211027$ eV, $E_2 = 0.0830912$ eV) and ($E_1 = 0.02872$ eV, $E_3 = 0.1799534$ eV), respectively. The abscissa of this point is the root $V_2^{\rm sol} = 0.235$ eV of $f_{E_1,E_2}(V_2) = f_{E_1,E_3}(V_2)$, and their ordinate is $V_1^{\rm sol} = 0.353$ eV determined by $V_1^{\rm sol} = f_{E_1,E_2}(V_2^{\rm sol})$ or $V_1^{\rm sol} = f_{E_1,E_3}(V_2^{\rm sol})$. The final step in the reconstruction is to determine the well width. From any of the Eqs. (4) we obtain $a = 13.5$ nm. Then, the well has been reconstructed exactly.

2.3. Symmetric potential well with known transition energies

To reconstruct a PW knowing the transition energies between the discrete energy levels is very important from the practical point of view because these transition energies are the ones experimentally measured [18, 19]. We show the case of a symmetric well, since this is the situation often met in practice. Let us consider the transition energies $\Delta E_{1,2} = E_2 - E_1$ and $\Delta E_{2,3} = E_3 - E_2$. Note that the energy $E_3 - E_2$ can be written as: $E_3 - E_2 = (E_3 - E_1) - (E_2 - E_1)$. This permits to write the transition $E_2 \leftrightarrow E_3$ in terms of the transition energies $E_1 \leftrightarrow E_2$ and $E_1 \leftrightarrow E_3$. We express the well width as a function of the barrier height and take the transition energy between two discrete levels as a parameter, for two different transitions. After, we seek for the well that has simultaneously the two transition energies. For E_1, E_2 and E_3 from (1) one gets

$$\frac{a\sqrt{2\mu E_n}}{\hbar} = n\pi - 2\arcsin\sqrt{\frac{E_n}{V}}, \qquad (7)$$

with $n = 1$, 2 or 3. The energy levels E_2 and E_3 can be expressed as a function of the energy level E_1 and the transition energies $\Delta E_{1,2}$ and $\Delta E_{1,3}$, by

$$\begin{aligned} E_2 &= E_1 + \Delta E_{1,2}, \\ E_3 &= E_1 + \Delta E_{1,3} \end{aligned} \qquad (8)$$

Substituting (8) into Eq. (7) and after some algebra we obtain:

$$\sqrt{1 + \frac{\Delta E_{1,k}}{E_1}} = \frac{k\pi - 2\arcsin\sqrt{\dfrac{E_1 + \Delta E_{1,k}}{V}}}{\pi - 2\arcsin\sqrt{\dfrac{E_1}{V}}}, \qquad (9)$$

where $k = 2$ or 3. The first equation in (7) can be written as

$$a = \frac{\hbar}{\sqrt{2\mu E_1}}\left(\pi - 2\arcsin\sqrt{\frac{E_1}{V}}\right). \qquad (10)$$

The transcendental Eqs. (9) can be expressed in the form

$$\Phi_{1,k}(V, E_1, \Delta E_{1,k}) = 0. \qquad (11)$$

In these equations the transition energies $\Delta E_{1,k}$ enter as parameters. This means that solving Eqs. (11) with V as the independent variable one gets all the energy levels E_1 coupled with the energy levels E_2 or E_3 through $\Delta E_{1,k}$. Next, we put into Eq. (10) the values of E_1 that satisfy Eqs. (11) for the corresponding V. By doing this, one finds all the PWs that contain the transition energy $\Delta E_{1,2}$ and all the PWs containing the transition $\Delta E_{1,3}$. Obviously, these PWs would be different. This can be expressed as:

$$a = f_{\Delta E_{1,2}}(V, E_1)$$

and

$$a = f_{\Delta E_{1,3}}(V, E_1). \qquad (11a)$$

The solution of the inverse problem will be completed when both Eqs. (11a) equal,

$$f_{\Delta E_{1,2}}(V, E_1) = f_{\Delta E_{1,3}}(V, E_1). \qquad (12)$$

The root $V_{\rm sol}$ of Eq. (12) is the barrier height of the PW, the well width a is obtained by evaluating any of the functions (11a).

Finally we show the method with a numerical example: Let us consider a PW with the transitions $\Delta E_{1,2} = 0.053$ eV and $\Delta E_{1,3} = 0.139$ eV corresponding to a PW with $a = 15$ nm and $V = 0.31$ eV, and suppose that we only know the values of the transitions $\Delta E_{1,2}$ and $\Delta E_{1,3}$. Figure 4 illustrates the situation. There, the transition energy $\Delta E_{1,2}$ as a function of the well width a for different V are plotted. The value of $\Delta E_{1,2}$ is also shown, see the horizontal line. The inset shows the graphic of Eq. (11a): $a = f_{\Delta E_{1,2}}(V, E_1)$. This curve represents the intersection of the family curves $\Delta E_{1,2}(a)$ with the experimental value of the transition en-

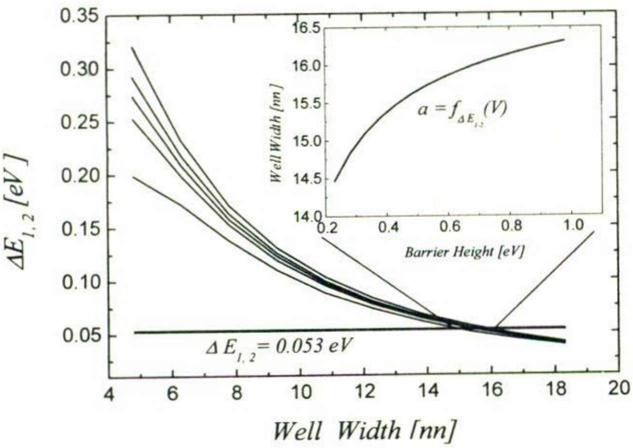

FIGURE 4. Dependence of the transition energy between $\Delta E_{1,2}$ *versus* well width a for different values of the barrier height V. The inset represents the locus of all the wells containing the transition energy $\Delta E_{1,2} = 0.056$ eV.

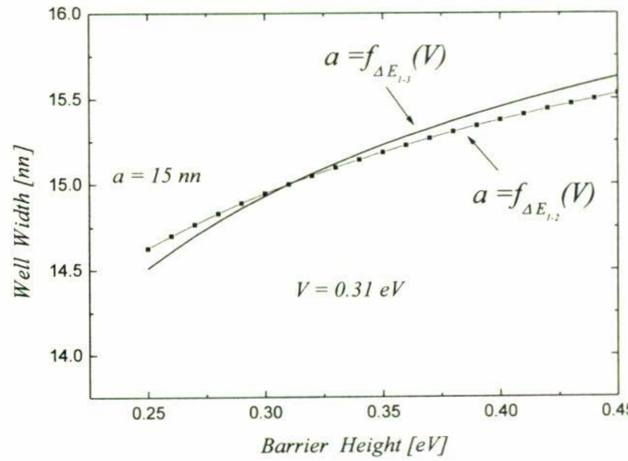

FIGURE 5. Graphic solution of Eq. (12). The intersection point $f_{\Delta E_{1,2}}(VE_1) = f_{\Delta E_{1,3}}(VE_1)$ gives the well width $a = 15$ nm and barrier height $V = 0.45$ eV.

ergy $\Delta E_{1,2} = 0.053$ eV. A similar family curves can be obtained for the transition energy $\Delta E_{1,3} = 0.139$ eV and the corresponding curve $a = f_{\Delta E_{1,3}}(V, E_1)$. The graphical solution of the inverse problem is demonstrated in Fig. 5 where $V_{\text{sol}} = 0.31$ eV and $a_{\text{sol}} = 15$ nm represent the intersection point of Eq. (12).

3. Conclusions

In this paper, we have developed a method for the reconstruction of rectangular PW (symmetric and asymmetric) provided the values of the energy levels are known. We also have shown how to restore a symmetric PW when the transition energies between the discrete energy levels are known from the experiment. This constitutes the case of major practical interest.

The method deduced in this article consists in expressing the well width a as a function of the barrier height V of the PW, using the values of the discrete energy levels or the transition energy between the discrete levels as parameters. After this, we found the PW for which all the conditions are fulfilled simultaneously. In the case of a symmetric PW it is sufficient to know two energy levels, while for the asymmetric PW three energy levels are needed. In this case the method of solution is more complicated but it is based on the same idea.

We think that the exercises shown in this paper can be included in the undergraduate courses of quantum mechanics, taking into account that nowadays the massive use of the PC in the university facilitates the tedious calculation characteristic to these methods.

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