Garrett approximation for asymmetric rectangular potentials and its applications to quantum well infrared photodetectors

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May 16, 2018

Abstract

Garrett’s approximation for the calculation of bound states energy in square wells is applied in a consistent way. So, one obtains simple formulas for these energies, with errors of about 1% for moderate, and 0.01% for deep wells. The application in of our results in the physics of quantum well infrared photodetectors is briefly discussed.

1 Introduction

The symmetric square well (Fig. 1), and more complicated rectangular wells (Figs. 2, 3, 4), are popular models of semiconductor heterojunctions potentials. The wave functions of particles moving in such potentials can be easily expressed in terms of elementary functions, but the bound states energy eigenvalues are given by transcendental equations, which defies exact solutions. However, several approximate analytic formulas of the eigenenergy were proposed. One of them, sometimes called the Barker approximation [1], has been successfully used to explain, inter alia, the optical absorption spectra of certain quantum wells / heterojunctions [2]. Powerful mathematical softs, giving accurate numerical results for the energy levels or any other quantity of interest, are available, but the attempt of finding an analytical solution, even an approximate one, remains appealing.

An interesting approach for obtaining analytical approximate expressions for the bound state energy of a particle in a square well was proposed by Garrett [3]. Unlike other approximations, obtained by various mathematical tricks applied to the transcendental eigenvalue equations [4, 5, 6, 7], Garrett’s method is based on a simple physical idea: as the main difference between the infinite and
finite square well is the fact that, in the first case, the wall is impenetrable, but in the second one, the wave function penetrates the wall on a certain distance $\delta$, the energy of a bound state in a finite well of length $L$ should be satisfactorily approximated by the energy of the corresponding bound state, in an infinite well of length $L + \delta$. Garrett also mentioned that the same approach could be applied to asymmetric wells. However, he did not apply this idea, not even for a symmetric square well. This simple exercise has been done recently in [5], [7], when it has been also shown that the Garrett approximation, obtained by a consequent application of Garrett’s idea, is equivalent to Barker’s approximation for deep wells.

As already mentioned, the square wells are not only a useful framework for discussing undergraduate problems of one-dimensional quantum mechanics: they have also important practical applications. One of them refers to the physics of semiconductor heterojunctions, characterized by various types of square wells. For the design and production of a class of quantum wells infrared photodetectors, it is essential to describe correctly the bound state energy in such piecewised defined potentials. We shall explain how Garrett’s approximation, in conjunction with other approximate analytical methods, can give quite accurately the energy levels of interest in the study of these devices.

The structure of this papers is the following: in Section 2, we obtain the Garrett approximation of the energy of bound states, in symmetric and asymmetric wells. In Section 3 we give the equation of the dimensionless wave vector of the bound states of an asymmetric well, mainly in order to estimate the errors of the Garrett approximation, for both symmetric and asymmetric wells. In Section 4, we show how the Garrett approximation can give simple and relatively accurate expressions of the energy levels relevant for the physics of quantum well infrared photodetectors. The last section is devoted to conclusions.

## 2 Garrett’s approximation for finite square wells

In order to expose Garrett’s approach, let us mention that the energy levels of a particle of mass $m$ in an infinite rectangular well of length $L$ is given by the well-known formula:

$$E_n^{(0)} = n^2 \frac{\pi^2 \hbar^2}{2mL^2}$$

(1)

The same particle, moving in a finite square well of depth $V$ and the same length $L$ (see Fig.1), can penetrate the wall of the well on a distance of about:

$$\delta^{(1)} = \frac{\hbar}{\sqrt{2m \left( V - E_n^{(0)} \right)}}$$

(2)

So, it behaves similarly to a particle moving in an infinite well of length $L + 2\delta^{(1)}$; consequently, its energy can be written as:
\( E_n^{(1)} = n^2 \frac{\pi^2 \hbar^2}{2m (L + 2\delta^{(1)})^2} \) \( (3) \)

which can be considered a first correction to (1). Using \( E_n^{(1)} \), we can define a new characteristic length:

\[ \delta^{(2)} = \frac{\hbar}{\sqrt{2m \left(V - E_n^{(1)}\right)}} = \frac{\hbar (L + 2\delta^{(1)})}{2mV (L + 2\delta^{(1)})^2 - \pi^2 \hbar^2 n^2} \] \( (4) \)

and we can define, similar to (2), a second correction to (1). A consistent application of this approach requests an infinity of steps, the general one being:

\[ \delta^{(q+1)} = \frac{\hbar (L + 2\delta^{(q)})}{2mV (L + 2\delta^{(q)})^2 - \pi^2 \hbar^2 n^2} \] \( (5) \)

Putting:

\[ \lim_{q \to \infty} \delta^{(q)} = \Delta, \quad y = \frac{2\Delta}{L} \] \( (6) \)

and taking the limit \( q \to \infty \) in the both sides of (6), we obtain a quartic equation in \( y \):

\[ 4P^2 y^4 + 8P^2 y^3 + (4P^2 - \pi^2 n^2 - 4) y^2 - 8y - 4 = 0 \] \( (7) \)

where \( P \) is the strength of the finite well:

\[ P = \sqrt{2mV L} \frac{\hbar}{2} \] \( (8) \)

So, \( P \) is a dimensionless quantity, characterizing both the potential \((L, V)\) and the particle \((m)\).

If the well is large, the cubic and quartic terms in eq. (7) can be neglected, and one obtains:

\[ y \simeq \frac{1}{P} + \frac{1}{P^2}, \quad \Delta = \frac{L}{2} \left( \frac{1}{P} + \frac{1}{P^2} \right) \] \( (9) \)

and the energy of the \( n \)-th bound state in the finite well can be approximated by:

\[ E_n = n^2 \frac{\pi^2 \hbar^2}{2m (L + 2\Delta)^2} = n^2 \frac{\pi^2 \hbar^2}{2mL^2 \left(1 + \frac{1}{P} + \frac{1}{P^2}\right)^2} \] \( (10) \)

Also, as \( 2mE_n = \hbar^2 k_n^2 \),

\[ Lk_n = \frac{\pi n}{1 + \frac{1}{P} + \frac{1}{P^2}} \] \( (11) \)
So, in this approximation, the quantity $Lk_n$, called sometimes dimensionless wave vector, depends linearly on $n$.

Let us remind that the equation giving the exact values of the wavevectors $k_n$ is [8], [9]:

$$n\pi - kL = 2 \arcsin \frac{kL}{P}$$

(12)

A plot of the bound state energies given by the solutions of the exact equation (12) and by the Garrett approximation (10) is given in Fig. 5.

For a simple asymmetric square well (see Fig. 2), we expect, for the same physical reasons as for a symmetric one, that, instead of (11), the dimensionless wave vector will be given by:

$$Lk_n = \frac{\pi n}{1 + \frac{1}{2} \left( \frac{1}{P_1^2} + \frac{1}{P_2^2} \right) + \frac{1}{2} \left( \frac{1}{P_2^2} + \frac{1}{P_2^2} \right)}$$

(13)

where we put:

$$P_i = \sqrt{2mV_i} \frac{L}{2\hbar}, \quad i = 1, 2$$

(14)

We shall call formulas (11), (12) Garrett approximations for the symmetric, respectively asymmetric wells. Even if Garrett did not obtain these formulas explicitly, he gave the intuitive idea of this new and simple approximation. It is more convenient to use the formulas for the wave vector than that for energy, for instance (11) instead of (10), as they are linear in $n$. For deep wells, $P \gtrsim 10$, the Garrett approximation is equivalent to Barker’s one [1].

The ground state dimensionless wave vector $Lk_1$ of the symmetric square well, given by the "exact" solution of the eigenvalue equation (disks) and by the Garrett approximation (squares), for strength $P = 1, 2, ..., 15$, are plotted in Fig. 6. For shallow wells ($P \leq 3$), the approximation is poor (about 10%), but for moderate ($4 \leq P \leq 9$) and deep ($10 \leq P$) wells it is of the order $10^{-2}$, respectively $10^{-3}$.

3 The simple asymmetric well

Let us consider the simplest generalization of the symmetric well (Fig. 2), called sometimes symple asymmetric square well. Its corresponding Schroedinger equation:

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi = E\psi$$

(15)

can be written simpler, as

$$\psi'' + [k^2 - U(x)] \psi = 0$$

(16)

if we introduce $U(x)$ instead of $V(x)$ by:
We shall define, following Messiah [9], Ch. III, §6 (see also [8], §22, problem 2)

\[ U(x) = U_3 \Theta (b-x) + U_2 \Theta (x-b) \Theta (a-x) + U_1 \Theta (x-2) \] (18)

The bound state wave functions have the form:

\[ \psi(x) = \begin{cases} 
A_1 e^{-K_1 x}, & x > a \\
A_2 \sin (kx + \varphi), & b < a < a \\
A_3 e^{K_3 x}, & x < b 
\end{cases} \] (19)

We shall put:

\[ k = \sqrt{k^2 - U_2}, \quad K_1 = \sqrt{U_1 - k^2}, \quad K_3 = \sqrt{U_3 - k^2} \] (20)

Without restricting the generality, we can choose \( U_2 = 0 \) and define:

\[ L = b - a, \quad U = U_1, \quad U_3 = (1 + \delta) U, \quad \delta > 0 \] (21)

Coming back to the general case, we get:

\[ K_1 = \sqrt{U - k^2}, \quad K_3 = \sqrt{(1 + \delta) U - k^2} \] (22)

The eigenvalue equation associated to the solution (19) has the form:

\[ n\pi - Lk = \arcsin \frac{Lk}{2P \sqrt{(1 + \delta)}} + \arcsin \frac{Lk}{2P} \] (23)

For a symmetric well, \( \delta = 0 \) and it becomes:

\[ n\pi - Lk = 2 \arcsin \frac{Lk}{2P} \] (24)

The relative errors of the Garrett approximation of the dimensionless wave vectors \( Lk \) whose exact value are given by the eqs. (23), (24) are plotted in Fig. 7; the approximation is more precise for an asymmetric well than for a symmetric one with the same strength, and decreases if the asymmetry increases.

The explanation of this behaviour is simple. Physically, an asymmetric wall is less penetrable than a symmetric one, of the same strength; in other words, it produces a stronger confinement effect. Mathematically, the function entering in the r.h.s. of (24), \( \arcsin x \), exists for \( x < 1 \); the function entering in the r.h.s. of (23), \( \arcsin x + \arcsin \frac{Lk}{\sqrt{1 + \delta}} \), exists for a shorter interval, \( x < (1 + \delta)^{-1/2} \). As

\[ \arcsin x = x + \frac{1}{6} x^3 + O(x^5), \]

a shorter interval favorizes the linear approximations - in our case, Garrett approximation. This is illustrated by Fig. 8, which gives the graphical solutions
It is clear that, for deep wells, the approximate solution is very close to the exact one. The accuracy of the approximation is also favored by the fact that its error changes its sign for bound states situated in the upper half of the well.

4 Applications to quantum well infrared photodetectors (QWIP)

The use of symmetric QW as photodetectors is hampered by the fact that, due to the symmetry of wave functions - in other words, to the existence of even and odd states - the selection rules forbid some photoabsorption processes. If the QW is asymmetric, such selection rules are no longer active, and the photoabsorption is enhanced [10]. In the last two decades or so, much work has been done on the effects of the asymmetry on optical and electrical properties of the detectors. Of course, the greatest interest is connected to infrared detectors, with important applications in imaging, pollution monitoring, spectroscopy of genes, etc. [11].

Such applications were studied by Brandel et al. [12], whose infrared detector is composed by thin quantum wells \((L = 20\,\text{A})\) of pure and doped \(\text{GaAs}\), sandwiched between thick \(\text{Al}_x\text{Ga}_{1-x}\text{As}\) barriers \((L_b = 300\,\text{A})\). More exactly, the QW is composed by two thin films, one of \(\text{GaAs}\) and the other of \(\text{Al}_y\text{Ga}_{1-y}\text{As}\), \(y < x\). As the films have slightly different compositions, there is a certain dif-
Figure 2: Simple asymmetric square well

Figure 3: Stepped square well with symmetric barriers
Figure 4: Stepped square well with asymmetric barriers

Figure 5: Dimensionless bound states wave vectors for a symmetric square well with $\gamma = 10$, given by the "exact" solution of the eigenvalue equation (disks) and by the Garrett approximation (squares)
Figure 6: Dimensionless ground state wave vector of the symmetric square well, given by the "exact" solution of the eigenvalue equation (disks) and by the Garrett approximation (squares), for P=1, 2, ...15.

The difference between the energy offsets, and they form a stepped asymmetric well ([12], Fig. 1), with enhanced photodetectivity. For a well with \( L = 40\,\text{A} \) and \( V = 1\,\text{eV} \), the potential strength is \( P \approx 5 \), (we approximated the effective electron mass inside the well with the free electron mass) characterizing a moderately deep well, when the error of Garrett approximation is \( \sim 1\% \). As \( 1\,\text{eV} \) is the energy corresponding to an infrared photon, \( \lambda = 1, 24\mu \), and interband transitions involve energies of a fraction of \( \text{eV} \), photodetectors similar to those described in [12] can be used in the near and mid-infrared region of spectra, and their characteristics can be calculated with reasonable accuracy using Garrett’s approximation.

Also, in this case, the penetration length is of the order

\[
\Delta = \frac{a}{2P} = 4\,\text{A},
\]

much smaller than the dimension of the barrier (\( L_b = 300\,\text{A} \)); the overlap of wave functions of neighbor wells is negligible, so the wells can be considered as decoupled.

If the relative doping of the thin films inside the barrier is small, \( y \ll 1 \), which happens when the main role of the step is to create asymmetry, so to enhance the photon absorption, the first-order perturbation theory to the levels of a symmetric well, given by very precise analytical approximations, will give errors of the order \( y \) for the energy levels of the stepped well. Indeed, in a
Figure 7: Error of Garrett approximation, in units of 0.1 percent, for the dimensionless bound state wave vectors of a simple asymmetric well with $\nu=10$ and $\delta=1/2$ (disks), $\delta=1$ (squares, edges parallel to axes) and $\delta=2$ (squares, diagonals parallel to axes); also, for $\delta=0$ (triangles).

Figure 8: Graphical solutions of the eq.(23).
slightly doped GaAs asymmetric stepped quantum well, the band discontinuity is \( \Delta = 0.8y \) (in eV) \( \text{[11]} \). A similar asymmetric well characterizes the device studied by Dupont et al. \( \text{[11]} \), for generating coherent terahertz waves.

Hostut et al. \( \text{[13]} \) studied a tri-colour infrared photodetector, obtained by repeated layers of three GaAs QW units. In each unit, the wells are thin GaAs layers (\( \sim 50A \)) separated by thick \( Al_xGa_{1-x}As \) barriers (\( L_b = 300A \)). The wells are simple asymmetric wells, with a small asymmetry, see Fig. 1 of \( \text{[13]} \). For this type of photodetector, the transition from the ground state of the well to the highest state is of interest; if the parameters of the detector are adapted to near- or mid-infrared region, the wells are quite deep (\( P \sim 10 \)), so Garrett approximation would be appropriate for calculation of the ground state energy.

5 Conclusions

Following in a consistent manner Garrett’s idea to approximate the bound states energy of a finite square well by the energy of the corresponding state of a conveniently defined infinite well, we obtain simple formula for the levels of symmetric and asymmetric wells, with errors of about 1\% for moderate, and about 0.1\% for deep wells. In this way, we can calculate, with reasonable approximation, the energy levels of QW, relevant for the physics of quantum well infrared photodetectors. It is quite surprising that such a simple approach works in a problem governed by complicated and untractable eigenvalue equations. The results can be applied to stepped wells, using elementary perturbation theory of quantum mechanics, at least in the case of small concentrations of dopants.

Acknowledgement 1 The author acknowledges the financial support of the ANCSI - IFIN-HH project PN 18 09 01 01/2018.

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