

# UPPER AND LOWER BOUNDS TO EIGENVALUES FROM SQUARE STEP POTENTIALS

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## ABSTRACT

A very simple method to obtain rough analytical upper and lower bounds to eigenvalues of one-dimensional quantum-mechanical models with potentials that are bounded from below is presented. The procedure is based on the properties of the eigenvalues of Hamiltonians with square step potentials and also provides the correct behaviour of the eigenvalues in the large quantum number limit.

## RESUMEN

Se presenta un método simple para obtener cotas superiores e inferiores para los autovalores de modelos mecano-cuánticos unidimensionales cuyos potenciales están acotados inferiormente. El procedimiento se basa en las propiedades de los autovalores de hamiltonianos con potenciales escalonados y proporciona también el comportamiento correcto de los autovalores en el límite de grandes números cuánticos.

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## 1. INTRODUCTION

Since the Schrödinger equation can be solved only for a few quantum-mechanical models, the eigenvalues of most problems of real physical interest are to be obtained through approximation methods. The variational procedure, which is frequently used in this type of approximate calculations, yields upper bounds to the eigenvalues when certain conditions are satisfied.

The accuracy of the computed eigenvalues can be assured only after obtaining proper upper (UB) and lower bounds (LB) to the exact ones. For this reason, several expressions that provide analytical UB and LB to eigenvalues were reported in recent years. In what follows, we discuss some of them using the  $k$ -oscillator model,

$$H = -d^2/dx^2 + |x|^k, \quad (1)$$

as an example.

Recently, Crandall and Reno<sup>(1)</sup> have shown that

$$E_0^U = \{(k/2)\sin(\pi/k)\}^{2k/(k+2)} \quad (2)$$

and

$$E_0^L = \sup_{0 < z < \pi/2} (z^k \cot^2 z)^{2/(k+2)} \quad (3)$$

are good UB and LB, respectively, to the ground-state eigenvalue of (1) when  $k > 2$ . The first bound is exact in the limits  $k \rightarrow 2^+$  and  $k \rightarrow \infty$ . For  $k < 2$ , a good UB is provided by the expectation value of the Hamiltonian (1)<sup>(1)</sup>:

$$E_0^U = \langle \Psi | H \Psi \rangle = \{\Gamma(k/(k+2))/\Gamma(2/(k+2))\} \{k(k+2)^k / 2^{2k+1}\}^{2/(k+2)}, \quad (4)$$

where

$$\Psi = N_k \exp \{-(2k)^{1/2} |x|^{1+k/2}/(k+2)\} .$$

The bound (4) is exact for  $k=2$  and in the limit  $k \rightarrow 0^+$ .

Lower bounds to the ground state of (1) when  $k < 2$  can be obtained from the Barnsley's method<sup>(2)</sup>:

$$E_0^L = \inf_{x>0} \frac{H\Psi}{\Psi} . \quad (6)$$

On using the wavefunction (5), the LB (6) is found to be<sup>(1)</sup>

$$E_0^L = (k/8)^{k/(k+2)} (1 + k/2) . \quad (7)$$

This bound is exact in both limits  $k \rightarrow 0^+$  and  $k \rightarrow 2^-$ .

The purpose of this paper is to develop a simple and useful procedure for obtaining UB and LB to the eivengalues of one-dimensional quantum-mechanical models. Though our bounds are not as accurate as those discussed in Ref. 1 when applied to the  $k$ -oscillator model, they exhibit clear advantages: (i) they can be obtained easily; (ii) they hold for any state; and (iii) they give us the correct quantum-number dependence of the eigenvalues in the large quantum-number limit.

The method is presented in Section 2 and the computed UB and LB to the ground state of (1) are compared with (2), (3), (4) and (7) in Section 3.

## 2. THE METHOD

Let us consider the eigenvalues equation

$$H\Psi_n = E_n \Psi_n , \quad (8a)$$

where

$$H = -d^2/dx^2 + V(x) . \quad (8b)$$

Our procedure can be applied to any one-dimensional interaction potential that holds at least one bound state, but in order to simplify the following discussion we restrict ourselves to consider even potentials only:

$$V(x) = V(-x) . \quad (8c)$$

Besides, we suppose that  $V(x)$  is a monotonic increasing function of  $|x|$ .

The eigenvalues of the Schrödinger equation

$$H^U \psi_n^U = E_n^U \psi_n^U, \quad H^U = -d^2/dx^2 + V^U(x), \quad (9a)$$

where

$$V^U(x) = V(a) \quad \text{if} \quad |x| \leq a \quad (9b)$$

and

$$V^U(x) = \infty \quad \text{if} \quad |x| > a, \quad (9c)$$

are UB to  $E_n$  because  $V^U(x) > V(x)$  for all  $x$  values. The best UB is obtained when  $E_n^U$  attains its minimum value. Choosing  $a = a_n$  in order to satisfy this condition, we have

$$E_n^U = (n+1)^2 \pi^2 / (4a_n^2) + V(a_n) > E_n \quad (n = 0, 1, 2, \dots), \quad (10a)$$

where

$$a_n^3 = (n+1)^2 \pi^2 / \{2V'(a_n)\}, \quad V'(x) = (dV/dx)(x). \quad (10b)$$

On the other hand, the eigenvalues of

$$H^L \psi_n^L = E_n^L \psi_n^L, \quad H^L = -(d^2/dx^2) + V^L(x), \quad (11a)$$

where

$$V^L(x) = V(0) \quad \text{if} \quad |x| \leq a \quad (11b)$$

and

$$V^L(x) = V(a) \quad \text{if} \quad |x| > a, \quad (11c)$$

are LB to  $E_n$  because  $V^L(x) < V(x)$  for all  $x$  values. Since  $E_n^L < E_n$  for all  $a$  and  $n$  values, we can choose the  $a$  value ( $a = a_n$ ) in order to make  $E_n^L$  as large as possible. Due to the simple form of the potential (11 b,c), the eigenvalues  $E_n^L$  can be easily computed<sup>(3)</sup>:

$$y_n \tan(y_n + p\pi/2) = (q^2 - y_n^2)^{\frac{1}{2}}, \quad p = \{1 - (-1)^n\}/2 \quad (n = 0, 1, \dots), \quad (12a)$$

$$q^2 = a^2V(a) \quad , \quad y_n^2 = a^2E_n^L \quad . \quad (12b)$$

When applied to the model (1), Eq. (10) leads to

$$E_n^U = \{(k+2)/2\} \{\pi^2(n+1)^2 / (2k)\}^{k/(k+2)} \quad . \quad (13)$$

From previous WKB results<sup>(4)</sup> we know that  $E_n \propto n^{2k/(k+2)}$  when  $n$  is large enough. Then, we can conclude that our UB exhibits the proper  $n$  dependence in the large  $n$  regime. Furthermore, this dependence is exact for all  $n$  values when  $k = -1, 2$  and  $\infty$ . This is a very suggestive fact because these are just the only problems of the form (1) for which the exact solutions are known.

Lower bounds to the eigenvalues of Hamiltonian (1) are obtained easily by replacing  $V(x) = |x|^k$  in Eq. (12). A straightforward calculation yields

$$E_n^L = y_n^{2k/(k+2)} |\cos(y_n + p\pi/2)|^{4/(k+2)} \quad , \quad (14a)$$

$$a_n = \{y_n / |\cos(y_n + p\pi/2)|\}^{2/(k+2)} \quad , \quad (14b)$$

$$y_n = (n-p/2)\pi + \tan^{-1}(\{q^2/y_n^2 - 1\}^{1/2}) \quad . \quad (14c)$$

In order to be a solution of (14c),  $y_n$  has to obey the inequality

$$n\pi/2 < y_n < (n+1)\pi/2 \quad . \quad (15)$$

From Eqs. (14a) and (15) it follows immediately that

$$E_n^U > E_n^L > (n\pi/2)^{2k/(k+2)} \quad . \quad (16)$$

Eqs. (13) and (16) are analytical UB and LB, respectively, to the eigenvalues of (1) and clearly show that  $E_n$  has to grow as  $n^{2k/(k+2)}$  in the large  $n$  regime. Besides, our UB and LB give us the exact result when  $k \rightarrow \infty$  and  $k \rightarrow 0$ :

$$\lim_{k \rightarrow \infty} E_n^U = \lim_{k \rightarrow \infty} E_n^L = (n+1)^2 \pi^2 / 4 \quad , \quad (17)$$

$$\lim_{k \rightarrow 0} E_0^U = \lim_{k \rightarrow 0} E_0^L = 1 \quad . \quad (18)$$

Then, these bounds will be better for very large and very low  $k$  values.

### 3. RESULTS AND DISCUSSION

In Table I, our UB and LB are compared with those obtained by means of Eqs. (2), (3), (4) and (7) for the ground state of (1). As stated before, our results are quite a rough approximation to the exact eigenvalues but the accuracy is markedly improved when  $k$  grows.

Although our bounds are not as accurate as the other ones, our method exhibits clear advantages for it is easy to apply to more complicated (bounded from below) one-dimensional potentials. Besides, it gives us only one analytical expression for all eigenvalues, whereas Eqs. (2), (3), (4) and (7) are bounds to  $E_0$  only. The procedure can also be used to obtain UB and LB to the eigenvalues of multidimensional systems, provided their potentials are bounded from below. For example, it could be powerful to deal with coupled anharmonic oscillators, these models being of great importance in the study of the vibrational motions of polyatomic molecules.

The accuracy of our bounds may be largely improved by increasing the number of steps in  $V^U$  and  $V^L$ , but in this way the number of variational parameters as well as the difficulties of the calculation of  $E^U$  and  $E^L$  also grows.

In its present form the method just described is very useful because it not only yields UB and LB to the magnitudes of all the eigenvalues of the model under consideration but also gives bounds to the growing rate of them. By this we mean that

$$\lim_{n \rightarrow \infty} E_n^B / E_n = \text{constant} \neq 0, \quad B = L, U. \quad (19)$$

Finally, we want to stress that our method may also be useful to calculate the number of bound states of a given potential. This knowledge is of great importance in several branches of Physics<sup>(5)</sup>.

TABLE I

k	$E_0^L$ <sup>a</sup>	$E_0^U$ <sup>a</sup>	$E_0^L$ <sup>b</sup>	$E_0^U$ <sup>c</sup>	$E_0^L$ <sup>d</sup>	$E_0^U$ <sup>e</sup>
0.05	0.892	1.146			0.906	1.055
0.1	0.826	1.264			0.852	1.078
0.5	0.615	1.976			0.750	1.078
1	0.554	2.554			0.854	1.029
2	0.561	3.142		1	1	1
5	0.732	3.467	0.781	1.733		
10	0.998	3.331	1.010	2.065		
16	1.227	3.163	1.231	2.206		
32	1.577	2.926	1.578	2.333		
64	1.881	2.750	1.881	2.399		
128	2.105	2.635	2.105	2.433		
256	2.253	2.2564	2.253	2.450		
1024	2.399	2.491	2.399	2.463		

<sup>a</sup> present calculation

<sup>b</sup> Eq. (3)

<sup>c</sup> Eq. (2)

<sup>d</sup> Eq. (7)

<sup>e</sup> Eq. (4)

Table I. Upper and lower bounds to the eigenvalues of the k-oscillator model (1).

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