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Quantum bouncer in a closed court

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The study of the quantum bouncer in a closed court is used to illustrate some concepts and techniques of quantum mechanics at different levels.

I. INTRODUCTION

The example of the quantum bouncer, which is a point mass falling in a uniform gravitational field and bouncing elastically on a flat horizontal floor, was proposed as a conceptual aid at the introductory level.[1] In the present paper we introduce the quantum bouncer in a closed court, which differs from the previous system by the presence of a flat horizontal ceiling where the point mass can also bounce off elastically. The ball game in the closed court can be made as interesting as in the open court. In fact, we use it to illustrate some concepts and techniques of quantum mechanics at different levels.

In Sec. II, we examine two alternative ways of solving the Schrödinger equation for the bouncer in a box. The first one coincides with that of Ref. 1, and the comparison of the solutions of both situations, closed versus open courts, is useful at the introductory level to illustrate the importance of the modified boundary condition. Of course, now both Airy functions have to be included. However, some eigenfunctions and energy eigenvalues can be easily obtained in terms of either Airy function and its zeros, and they can be incorporated in a geometric construction of the lowest energy curves for different heights of the ceiling. The second way of solving the problem consists in constructing and diagonalizing the matrix of the Hamiltonian of the system, for which we use the orthonormal basis of eigenfunctions for the free particle in a box. The matrix method,[2] usually studied in the second half of a regular course in quantum mechanics can be directly applied in this case. Numerical results and limits on their convergence and accuracy, owing to the truncation of the basis, can be obtained with the aid of a computer.

In Sec. III, we obtain some approximate solutions for the quantum bouncer in a box. The first one is based on perturbation theory,[2] using the free-particle in a box as the nonperturbed system and the linear potential as the perturbation; therefore, it can be directly constructed from the matrix elements previously obtained and it is expected to be valid for small boxes, i.e., low ceilings. The second one is an asymptotic solution valid for large boxes, i.e., high ceilings, and we construct it from the exact solution using the asymptotic forms of the Airy functions.

Some illustrative numerical results of the different solutions studied in this paper are presented in Sec. IV. A comparison of the exact and approximate solutions permits us to ascertain the ranges of validity of the latter.

In Ref. 1 and in Sec. II A, the Airy functions are directly taken from available tables,[3] which are appropriate for students at the introductory level. However, students at a more advanced level may be interested in studying the analytical forms of the Airy functions. With such students in mind we include an Appendix dealing with the explicit construction of the integral representations of these functions. Our treatment is based on the solution of the Schrödinger equation in the momentum representation.[2]

II. EXACT SOLUTIONS OF THE EIGENVALUE PROBLEM

The potential energy for the boxed-in bouncer is given by

$$V(y) = \begin{cases} \infty & y = 0 \\ mgy & 0 < y < y_0 \\ \infty & y = y_0, \end{cases} \tag{1}$$

where y_0 is the height of the ceiling. Then the stationary states of the quantum bouncer in the closed court are determined by the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dy^2} + mgy\right)\Psi(y) = E\Psi(y), \tag{2a}$$

subject to the boundary conditions

$$\Psi(y = 0) = 0, \tag{2b}$$

$$\Psi(y = y_0) = 0. \tag{2c}$$

It is useful to introduce the characteristic length

$$l = (\hbar^2/2m^2g)^{1/3}$$

and the dimensionless height and energy

$$z = y/l, \quad \epsilon = E/mgl.$$

A. Airy equation

We follow Ref. 1 in using the dimensionless coordinate $x = z - \epsilon$ and reducing Eq. (2a) to the Airy equation

$$\left(\frac{d^2}{dx^2} - x\right)\Psi(x) = 0$$

with the general solution

$$\Psi(x) = M\,Ai(x) + N\,Bi(x).$$

The boundary conditions, Eqs. (2b) and (2c), become

$$\Psi(x = -\epsilon) = 0 = M\,Ai(-\epsilon) + N\,Bi(-\epsilon),$$

$$\Psi(x = z_0 - \epsilon) = 0 = M\,Ai(z_0 - \epsilon) + N\,Bi(z_0 - \epsilon),$$

which can be viewed as a system of two linear homogeneous algebraic equations for the unknown coefficients M and N. Such a system can have a solution different from the trivial one $M = N = 0$, only if its determinant vanishes, i.e.,

$$\begin{vmatrix} Ai(-\epsilon) & Bi(-\epsilon) \\ Ai(z_0 - \epsilon) & Bi(z_0 - \epsilon) \end{vmatrix} = 0. \tag{3}$$

For a given height of the ceiling, or z_0, this equation can be

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satisfied only for discrete values of ϵ, which are the energy eigenvalues. For each of these eigenvalues, the ratio of the coefficients M and N is fixed by either of the boundary condition equations, which in turn determines the eigenfunction. Thus the solution of the eigenvalue problem is reduced to the numerical solution of Eq. (3).

Obviously, the open court situation of Ref. (1) can be recovered from our solution in the limit $z_0 \to \infty$, which requires $N = 0$ because of the divergent behavior of $Bi(z_0 - \epsilon)$.

Actually, some particular solutions of the quantum bouncer in the closed court can be easily constructed based on the zeros of one or the other of the Airy functions. Let us consider first those solutions with $N = 0$, then the boundary condition equations become

$$Ai(-\epsilon) = 0, \quad Ai(z_0 - \epsilon) = 0.$$

Therefore, these solutions are possible when the energy is the negative of one of the zeros of the Airy function and the height of the ceiling is the difference between two of those zeros,

$$\epsilon = -a_n, \quad z_0 = a_{n'} - a_n. \tag{4a}$$

Similarly, for $M = 0$, the solutions involve the zeros of the other Airy function, which are related to the energy and height by

$$\epsilon = -b_n, \quad z_0 = b_{n'} - b_n. \tag{4b}$$

We use Eqs. (4a) and (4b) to construct Fig. 1, which gives the variation of the lowest energy eigenvalues as a function of the height of the ceiling. Our construction starts from the graphs of the Airy functions $Ai(x)$, $Bi(x)$ shown on the left[3]; actually, only the positions of their zeros are needed and they are projected on the energy axis. The straight line through the origin and with slope one corresponds to the potential energy at the ceiling. Next, from each of the zeros of the Airy functions on the energy axis we draw straight lines with slopes zero and one, using dashed lines for $Ai(x)$ and dashed-dotted lines for $Bi(x)$. The intersections of one set of lines or the other in the first quadrant of the (z_0, ϵ) plane satisfy the conditions of Eqs. (4a) or Eqs. (4b), respectively. Consequently, such intersections belong to the energy curves and will serve as a reference for the tracing of the latter. Actually, this can be done fairly easily and directly by interpolation between successive intersections of the same order along the horizontals, in the region above the potential energy line. The portions of the Airy functions corresponding to the eigenfunctions of the particular states under consideration can be immediately identified on the left graph of Fig. 1. It is illustrative to verify graphically that they satisfy the boundary conditions and that their number of interior nodes equals the order of their excitation.

B. Matrix of the Hamiltonian

Another way of solving the Schrödinger equation [Eq. (2a)],

$$\left(-\frac{d^2}{dz^2} + z\right)\Psi(z) = \epsilon\Psi(z),$$

consists in writing the wave function as a linear combination of a complete set of orthonormal functions that satisfy the boundary conditions [Eqs. (2b) and (2c)],

$$\Psi(z) = \sum_{k=1}^{\infty} c_k \sqrt{\frac{2}{z_0}} \sin\frac{\pi k z}{z_0}. \tag{5}$$

The Fourier sine basis corresponds to the eigenfunctions of the free-particle in a box. Now, the problem is reduced to the determination of the expansion coefficients c_k. This can be accomplished by substituting Eq. (5) in the Schrödinger equation, and making use of the orthonormality of the basis functions to obtain a system of linear homogeneous algebraic equations for the unknown c_k's. Such a system has nontrivial solutions only if the determinant of its coefficients vanishes, which will occur only for discrete values of the energy.

The above is equivalent to the construction of the matrix of the Hamiltonian

$$\begin{aligned} H_{kk'} &= \left\langle k \left| \left(-\frac{d^2}{dz^2} + z\right) \right| k' \right\rangle \\ &= \frac{2}{z_0}\int_0^{z_0} \sin\frac{k\pi z}{z_0}\left(-\frac{d^2}{dz^2} + z\right)\sin\frac{k'\pi z}{z_0}\,dz \\ &= \left(\frac{k^2\pi^2}{z_0^2} + \frac{z_0}{2}\right)\delta_{kk'} + \frac{z_0}{\pi^2}\left(\frac{(-1)^{k-k'} - 1}{(k-k')^2} \right. \\ &\qquad \left. - \frac{(-1)^{k+k'} - 1}{(k+k')^2}\right)(1 - \delta_{kk'}) \end{aligned} \tag{6a}$$

and its subsequent diagonalization[2]

$$\det|(H_{kk'} - \epsilon\delta_{kk'})| = 0. \tag{6b}$$

In principle the expansion of Eq. (5) involves an infinite number of terms. In practice, the method has to be applied with a finite number of terms, i.e., the basis is truncated. In general, for a given number of terms the lower energy states are more accurately determined than the higher-energy ones. The convergence of the energy eigenvalues ϵ and the eigenfunction coefficients c_k can be tested by changing the number of terms included in the calculation.

Actually, an expansion of the type of Eq. (5) with a finite number of terms can be viewed also as a trial function in which the coefficients c_k are variational parameters. Then it is straightforward to show that the variational method leads to the same Eqs. (6a) and (6b).

III. APPROXIMATE SOLUTIONS

A. Perturbative solution

We construct a perturbative solution based on the Ray-

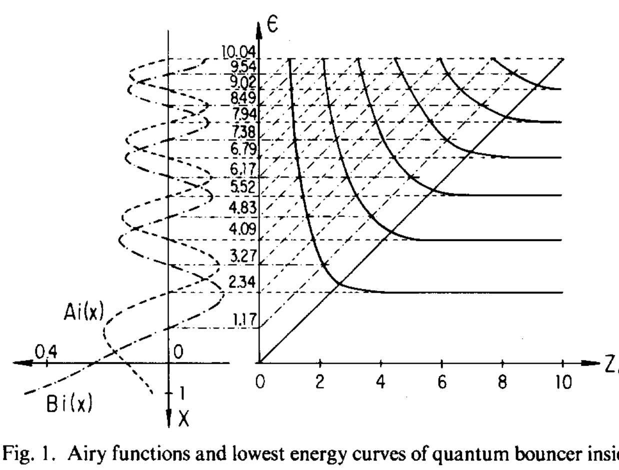

Fig. 1. Airy functions and lowest energy curves of quantum bouncer inside closed courts with different ceiling heights.

Table I. Lowest energy eigenvalues ϵ_i for different ceiling heights z_0.

z_0	1	2	4	6	8	∞
ϵ_1	10.368 507 2	3.449 867 6	2.355 495 2	2.338 134 9	2.338 107 4	2.338 107 41
ϵ_2	39.978 744 8	10.874 817 8	4.532 418 3	4.094 712 3	4.087 957 4	4.087 949 44
ϵ_3	89.326 634 5	23.209 728 2	7.600 776 5	5.662 858 0	5.521 663 5	5.520 559 83
ϵ_4	158.413 789 8	40.480 328 1	11.900 138 2	7.537 644 6	6.816 265 8	6.786 708 09
ϵ_5	247.240 189 3	62.686 296 5	17.441 563 3	9.956 836 6	8.168 262 6	7.944 133 59
ϵ_6	355.805 814 7	89.827 339 4	24.220 991 1	12.942 621 8	9.784 198 7	9.022 650 85
ϵ_7	484.110 657 4	121.903 323 0	32.236 351 9	16.487 858 5	11.729 550 6	10.040 174 34
ϵ_8	632.154 714 8	158.914 200 4	41.486 661 9	20.587 763 6	14.002 713 1	11.008 524 30

leigh–Schrödinger perturbation method,[2] taking the free particle in a box as the nonperturbed system. Consequently, the nonperturbed Hamiltonian is simply the kinetic energy and the perturbation is the linear potential. Using the respective matrix elements which appear explicitly in Eq. (6a), we can identify the lowest-order contributions to the energy eigenvalues:

$$\epsilon_k^{(0)} = \langle k|H_0|k\rangle = k^2\pi^2/z_0^2, \tag{7a}$$

$$\Delta\epsilon_k^{(1)} = \langle k|V|k\rangle = z_0/2, \tag{7b}$$

$$\Delta\epsilon_k^{(2)} = \sum_{k'\neq k} \frac{\langle k|V|k'\rangle\langle k'|V|k\rangle}{\epsilon_k^{(0)} - \epsilon_{k'}^{(0)}} = \left(\frac{z_0}{\pi^2}\right)^2 \frac{z_0^2}{\pi^2} \sum_{k'\neq k} \times\left(\frac{(-1)^{k-k'}-1}{(k-k')^2} - \frac{(-1)^{k+k'}-1}{(k+k')^2}\right)^2 \Big/ (k^2-k'^2). \tag{7c}$$

It is easy to verify that the ith-order contribution is proportional to z_0^{3i-2} resulting from the z_0^i and $(z_0^2)^{i-1}$ factors coming from the numerators and denominators, respectively.

For the ground state, $k = 1$, and the energy has the explicit perturbation expansion

$$\epsilon_1 = \frac{\pi^2}{z_0^2} + \frac{z_0}{2} - 0.001\,097\,26\, z_0^4 + \cdots, \tag{7d}$$

which is expected to be valid for small values of z_0, i.e., low ceilings. Naturally, higher-order contributions can also be calculated not only for the ground state but also for the excited states.

B. Asymptotic solution

In the case of very high ceilings, i.e., very large values of z_0, we can construct the corresponding solutions using the Taylor expansions and the asymptotic forms of the Airy functions for the upper and lower elements of the determinant in Eq. (3), respectively. The Taylor expansions have the argument $\epsilon + a_n = \delta \to 0$, because the energies tend asymptotically to their open court values for very high ceilings,

$$Ai(-\epsilon) = Ai(a_n) - \delta A'i\,(a_n) + \cdots \approx -\delta A'i\,(a_n), \tag{8a}$$

$$Bi(-\epsilon) = Bi(a_n) - \delta B'i\,(a_n) + \cdots \approx Bi(a_n). \tag{8b}$$

The asymptotic forms[3] are obtained from

$$Ai(x) = (1/2)x^{-1/4}\, e^{-\zeta} f(-\zeta), \tag{9a}$$

$$Bi(x) = x^{-1/4}\, e^{\zeta} f(\zeta), \tag{9b}$$

where

$$\zeta = (2/3)x^{3/2}$$

and

$$\lim_{\zeta\to\infty} f(-\zeta) = \lim_{\zeta\to\infty} f(\zeta).$$

Substituting Eqs. (8a) and (8b) and Eqs. (9a) and (9b) in Eq. (3), we obtain

$$\delta = -Bi(a_n)\, e^{-2\zeta_0}/2A'i\,(a_n) \tag{10a}$$

More explicitly,

$$\epsilon_n(z_0) = -a_n - \frac{Bi(a_n)}{2A'i\,(a_n)} e^{-(4/3)(z_0+a_n)^{3/2}}, \tag{10b}$$

showing how the asymptotic approach of the energy to its open court value is dominated by the exponential factor.

The bondary condition at the floor combined with Eqs. (8a) and (8b) gives the relative proportion of the Airy functions in the eigenfunction

$$\frac{N}{M} = \frac{\delta A'i\,(a_n)}{Bi(a_n)} = -\tfrac{1}{2}\, e^{-2\zeta_0}$$

showing the decreasing contribution of the irregular Airy function as the ceiling gets higher.

Table II. Comparison of the exact, perturbative, and asymptotic values of the ground-state energy for different ceiling heights z_0.

z_0	ϵ_1	ϵ_1 (pert.)	z_0	ϵ_1	ϵ_1(asymp.)
0.2	246.840 108 3	246.840 108 3	2.6	2.710 167 3	2.609 278
0.4	61.884 999 4	61.884 999 4	3	2.509 011 1	2.496 399
0.6	27.715 425 6	27.715 425 6	4	2.355 495 2	2.356 740
0.8	15.820 807 4	15.820 807 4	4.4	2.343 968 5	2.344 365
1.0	10.368 507 2	10.368 507 1	5	2.339 049 3	2.339 098 3
1.2	7.451 616 8	7.451 616 7	6	2.338 134 9	2.338 135 8
1.4	5.731 297 9	5.731 297 2	7	2.338 107 9	2.338 107 89
1.6	4.648 125 6	4.648 123 2	8	2.338 107 4	2.338 107 41
1.8	3.934 663 5	3.934 655 6	9	2.338 107 4	2.338 107 41
2.0	3.449 867 6	3.449 844 9			
2.2	3.113 529 1	3.113 470 5			
2.6	2.710 167 3	2.709 858 5			
3.0	2.509 011 1	2.507 744 6			

IV. NUMERICAL RESULTS AND DISCUSSION

A sample of numerical results for the exact and approximate solutions studied in Secs. II and III is presented in Tables I and II.

Table I contains the lowest energy eigenvalues obtained from the diagonalization of the matrix of the Hamiltonian, Sec. II B, for finite ceiling heights. For a given value of z_0, the diagonalization procedure yields the energy eigenvalues in the corresponding column. Such values can be taken as the exact ones up to the number of digits included, because they do not change when the dimension of the matrix is increased. Naturally, this dimension is much larger than 8 and has to increase for larger values of z_0. For the sake of completeness, we include in the last column of this table the asymptotic values of the energy eigenvalues, which correspond to those of the quantum bouncer in the open court, $-a_n$. Obviously, the values in this table can be used to complete Fig. 1, which we have done. The corresponding energy curves are monotonically decreasing as the height of the ceiling increases; their variation is dominated by the form $k^2z_0^{-2}$, Eq. (7a), for very small values of z_0, while they approach rapidly their asymptotic values, Eq. (10b), for not so large values of z_0, slightly larger than $-a_n$.

In Table II, we show the comparison of the exact numerical results with those from the perturbative solution, Eq. (7d), and the asymptotic solution, Eq. (10b), for low and high ceilings, respectively. From the left-hand side of the table we can see that the perturbative solution is indeed very good for very low ceilings and quite acceptable even for not so low ceilings. Similarly, the right-hand side of the table shows that the asymptotic solution is also very good for high ceilings and fairly reasonable for not so high ceilings. Here we have restricted our analysis to the ground state, but obviously it can be applied to the excited states, too.

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APPENDIX

The Schrödinger equation for the linear potential in the momentum representation[2] has the form

$$\left(\frac{p^2}{2m} + mgi\hbar\frac{d}{dp}\right)\Phi(p) = E\Phi(p). \qquad \text{(A1)}$$

The wave functions in the coordinate and momentum representations are related to each other through a Fourier transformation

$$\Psi(y) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{ipy/\hbar}\,\Phi(p)\,dp.$$

By comparing Eqs. (2a) and (A1) we see that the latter, being of first order, is easier to integrate. In fact, it is directly integrable and its general solution is

$$\Phi(p) = \Phi(0)e^{(1/i\hbar)(EP/mg - p^3/6m^2g)}. \qquad \text{(A2)}$$

The corresponding solution in the coordinate representation is

$$\Psi(y) = \frac{\Phi(0)}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{(1/i\hbar)[p(y-E/mg)+p^3/6m^2g]}\,dp$$
$$= \frac{2\Phi(0)}{\sqrt{2\pi\hbar}}\int_0^{\infty}\cos\left[p\left(y-\frac{E}{mg}\right)+\frac{p^3}{6m^2g}\right]dp, \qquad \text{(A3)}$$

where the last line is obtained from the previous one by dividing the integration interval into two portions, and in the first one from $-\infty$ to 0, the integration variable is changed from p to $-p$.

The square integrable wave function of Eq. (A3) can be identified with the regular Airy function as given by its integral representation

$$(3a)^{-1/3}\pi Ai[\pm(3a)^{-1/2}x] = \int_0^{\infty}\cos(at^3 \pm xt)\,dt.$$

On the other hand, the irregular Airy function with the integral representation

$$(3a)^{-1/3}\pi Bi[\pm(3a)^{-1/2}x] = \int_0^{\infty}[e^{-qt^3\pm xt} + \sin(at^3 \pm xt)]dt,$$

can not be directly obtained from Eq. (A3), because it is not square integrable in the entire interval $-\infty < x < \infty$. However, a combination of both Airy functions can be obtained from the first line of Eq. (A3) by changing the path of integration in the complex p plane from that of the real axis to one starting from $(0, -i\,\infty)$ to the origin along the negative imaginary axis and then going out to $(\infty, 0)$ along the positive real axis. It is easy to check that the real and imaginary parts of such an integral correspond to the regular and irregular Airy functions, respectively.

[a]On leave of absence from Instituto de Física, University of Mexico, Mexico, DF.

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"... Education should turn out the pupil with something he knows well and something he can do well. This intimate union of practice and theory aids both. The intellect does not work best in a vacuum. ..."

Alfred North Whitehead