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Energy eigenvalues and Einstein coefficients for the one-dimensional confined harmonic oscillators

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Abstract

We compute the energy eigenvalues and the Einstein coefficients for a one-dimensional harmonic oscillator confined in a box of impenetrable walls as a function of box size, and an asymmetry parameter. The energy eigenvalues that we obtain for the symmetric and unsymmetric confinement are more accurate than those reported previously. To compute eigenvalues and eigenfunctions we use two different approaches known to be very accurate. With respect to the unbounded harmonic oscillator we find transitions that are now allowed due to the confinement to the box. When the confinement is asymmetric the transition spectra become more complex, since the transition probabilities show a strong variation with box size.

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1. Introduction

The study of confined systems has been used for quite some time to understand different physical phenomena, such as the behaviour of systems under the action of an external high pressure [1]. In this sense one-dimensional models have provided a natural starting point to model the effects of confinement since they are quite simple, but nevertheless can display interesting behaviour without the need to resort to complex situations. For example, in a recent work, Bhattacharya and Mukhopadhyay [2] study the force $F(L) = -dE(L)/dL$ necessary to confine a particle in a one-dimensional box of length L , which at the same time is subjected to a potential which can be either a harmonic oscillator potential x^2 , or a pure anharmonic x^4 potential.

The harmonic oscillator can be confined in a symmetrical or an asymmetrical way inside a box. The first case is the most familiar and therefore is one of the most often studied models [1, 3–10]. It has been in vogue since the 1940s starting with the works by Kotari and Auluck [3], Auluck [4] and Chandrasekhar [5] as a model in the study of some properties of dense stars, white dwarfs and galactic clusters. It has also been used to analyse electric and magnetic properties [6], as well as the specific heat of metals under high pressure [7]. In one approach, the Schrödinger equation for the symmetrically confined harmonic oscillator was solved in terms of the Kummer function $M(a, b, z)$ [8]; imposing the boundary conditions one obtains a transcendental equation for the energy eigenvalues that must be solved numerically [9]. Other authors have solved the Schrödinger equation, for this symmetric case, following other approaches such as perturbation theory [8, 10–12], Padé approximants [8], direct diagonalization of the Hamiltonian [8], or using Numerov's method [13]. In view of all these works we see that the study of an asymmetrically confined one-dimensional harmonic oscillator has not been very common, even though in reality the asymmetric confinement should be more usually realized. In this case the Schrödinger equation is

$$\frac{1}{2} \frac{d^2 \psi}{dx'^2} + \left(E - \frac{1}{2} (x' - d)^2 + V(x') \right) \psi = 0, \quad (1a)$$

where

$$V(x') = \begin{cases} +\infty, & |x'| \geq R, \\ 0, & |x'| < R. \end{cases} \quad (1b)$$

Here, $2R$ is the length of the box and d is the location of the minimum of the harmonic oscillator potential. The distances are measured in units of $(\hbar/m\omega)^{1/2}$, and the energy unit is $\hbar\omega$. One of the first studies of this problem is due to Vawter [14], who developed an approximate solution using the WKB method. He found the values of the energy for two limiting situations:

- (i) for the lower states, where the classical turning points are located inside the well $E_n \simeq (n + \frac{1}{2})$, and
- (ii) for highly excited states, where the classical turning points of the oscillator are well outside the box, where the particle can no longer reach them, the approximate values are then $E_n \simeq [(n + 1)^2 \pi^2] / R^2$.

Vawter [14] also obtained the solution of Schrödinger equation (1) in the form of a power series expansion in x' and calculated the expansion coefficients from a recurrence relation, from which he determined the energy eigenvalues numerically. A different approach was employed by Fernández and Castro [15] who used the hypervirial formulae for enclosed quantum systems. Aquino *et al* [11] and Fernández [12] solve this problem using first- and second-order perturbation theory, respectively; both methods give results that are valid only for boxes with $R \leq 1.5$. The rest of this paper is organized as follows. In section 2 we present two different methods to solve the Schrödinger equation, and we obtain the energy eigenvalues for the symmetric and the asymmetric confined case. In section 3 we compute the Einstein coefficients for the confined harmonic oscillator as a function of the box size for both cases. Finally, in section 4 we present our conclusions.

2. The energy eigenvalues

We used two different methods to find the energy eigenvalues and eigenfunctions of the one-dimensional confined oscillators. The first method is based on a power series expansion of

the wavefunction itself [17–21], while the second one is completely numeric in nature [16] and is based on the Runge–Kutta method of integrating ordinary differential equations. The first method is very efficient when the values of the wavefunction and its derivative are well known at the origin, and it was successfully applied to the problem of a confined hydrogen atom [19, 21], a three-dimensional harmonic oscillator [20, 21], a two-dimensional confined hydrogen atom [21] and also in the study of the inversion of NH_3 [22] where the inversion potential was modelled by a polynomial of degree 20. The second method is more efficient for the study of asymmetric potentials, although it can also be applied to study systems with symmetrical potentials. It was also applied to compute the energy eigenvalues of the Mitra potential [16] and the inversion of PH_3 [23].

To keep the presentation of this work self-contained, but brief, we only mention the main characteristics of both methods. Clearly, in the original papers the reader can find more detailed explanations.

In order to solve the Schrödinger equation (1a) it is advisable to make the following change of variable:

$$x = x' - d. \quad (2)$$

Equation (1a) is then transformed to a Schrödinger equation for the harmonic oscillator centred at the origin:

$$-\frac{1}{2}\psi'' + \frac{1}{2}x^2\psi(x) = \epsilon\psi(x), \quad (3)$$

and the boundary conditions are now given by

$$\psi(a) = \psi(b) = 0, \quad (4)$$

where

$$a = -(R + d), \quad b = R - d. \quad (5)$$

One of the main features of the method is the assumption that ψ must be a function of both position and energy, i.e.

$$\psi = \psi(x, \epsilon). \quad (6)$$

The derivative of equation (3) with respect to the energy is given by

$$\partial\psi''/\partial\epsilon = [x^2 - 2\epsilon](\partial\psi/\partial\epsilon) - 2\psi. \quad (7)$$

Starting with an initial guess for the energy, (3) and (7) must be solved for ψ and $\partial\psi/\partial\epsilon$. The correction to the energy is obtained through the Newton–Raphson method [24, 25].

2.1. The symmetric confinement

In this case, $d = 0$ and equation (5) is then

$$a = -R, \quad \text{and} \quad b = R.$$

The symmetry of the problem simplifies the computation, since it is sufficient to consider only the wall on the right-hand side. The confinement of the system introduces an impenetrable barrier at $x_0 = b$ and, therefore, the function ψ must vanish there:

$$\psi(x_0, \epsilon_{\text{exact}}) \equiv 0. \quad (8)$$

The problem of finding the energy eigenvalues of equation (3) has now been reduced to finding the zeros of ψ with respect to ϵ at x_0 . One starts by making an initial guess for the energy, ϵ_i , equations (3) and (7), and then solving numerically to find ψ and $\partial\psi/\partial\epsilon$, respectively. A correction for the energy is then computed through the Newton–Raphson method [23, 24]:

$$\epsilon_{i+1} = \epsilon_i - \psi(x_0, \epsilon_i)/[\partial\psi(x_0, \epsilon_i)/\partial\epsilon]. \quad (9)$$

With this new value of the energy we iterate equations (3) and (7) until a final eigenvalue ϵ_f is found with the desired accuracy. In this approach the wavefunction is expressed as a Taylor series around $x = 0$, where its initial value is known:

$$\psi(x) = \sum_k T_k, \quad (10a)$$

where

$$T_k = (\psi^{(k)}(0)/k!)x^k. \quad (10b)$$

To evaluate this expression we take the p th derivative of equation (3) with respect to x and use the well-known formula for the derivative of a product, together with equations (10a) and (10b). Finally, we obtain that

$$T_p = x^2(T_{p-2}x^2 - 2\epsilon T_p)/[(p+1)(p+2)]. \quad (11)$$

Hence, the wavefunction can be calculated directly using (10a), and also $\partial\psi/\partial\epsilon$:

$$\partial\psi/\partial\epsilon = \sum_m \partial T_m/\partial\epsilon = \sum_p \dot{T}_p, \quad (12)$$

where \dot{T}_p denotes the derivative of T_p relative to the energy:

$$\dot{T}_p = x^2(\dot{T}_{p-2}x^2 - 2\epsilon\dot{T}_p - 2T_p)/[(p+1)(p+2)]. \quad (13)$$

Using equations (10)–(13) we can build any eigenstate using the initial conditions. Due to the symmetry of the system the states have a well defined parity. Then, for the even states $\psi_n(0) = 1$ and $\psi'_n(0) = 0$ and for odd states $\psi_n(0) = 0$ and $\psi'_n(0) = 1$. Once the energy eigenvalue ϵ_n has been obtained, we can compute the expansion coefficients for the wavefunction, substituting ϵ_n in equation (11) and evaluating T_p at $x = 1$. Thus, we have that

$$\psi_n(x) = \sum_m T_m(x = 1, \epsilon_n)x^m. \quad (14)$$

A major advantage of this method is that the computation of the energy eigenvalues is not only very accurate, but also quite fast. Table 1 shows the energy eigenvalues ϵ_n for ground state and first excited state for different values of the size of the box. We compare our results, for symmetric confinement, with those of Aguilera-Navarro *et al* [8], obtained by a direct diagonalization of the Hamiltonian in the basis set of a free particle in a box. Note that the results of [8] only provide good approximations for small boxes and only for the lowest states, but they become less accurate when the box size increases. This behaviour is easily observed for the states E_0 , E_1 , E_2 and E_3 ; at $R = 6$, the values reported [8] are lower than the exact ones for the free harmonic oscillator. With the method proposed here, it is possible to obtain the energy eigenvalues with a high degree of precision: all digits shown in table 1 are significant. The results reported in [13] agree with those of table 1 up to the first 9 digits after the decimal point and, therefore, showing that their results are also a good approximation. It can be observed that, for small box sizes, $R < 1.5$, all the energy levels are close to the respective energy eigenvalues of the free particle in a box of the same size [11]; in this case, the harmonic oscillator potential is just a perturbation. On the other hand, for $R > 5$ the energy levels approach the corresponding eigenvalues of the unconfined harmonic oscillator, as expected.

Table 1. Energy eigenvalues for the ground state and a few excited states of a symmetrically confined harmonic oscillator. The size of the box is $2a$, the length unit is $\sqrt{\hbar/m\omega}$ and the energy unit is $\hbar\omega$.

a	E_0 [8]	E_0 (ours)	E_1 [8]	E_1 (ours)
0.5	4.951 129 323 264	4.951 129 323 254 130	19.774 534 178 560	19.774 534 179 208 319
1.0	1.298 459 831 928	1.298 459 832 032 056	5.075 582 014 976	5.075 582 015 226 783
2.0	0.537 461 209 21	0.537 461 209 281 675	1.764 816 438 592	1.764 816 438 780 636
3.0	0.500 391 082 8	0.500 391 082 929 748	1.506 081 527 088	1.506 081 527 252 794
4.0	0.500 000 490 7	0.500 000 490 856 430	1.500 014 602 7	1.500 014 603 007 123
5.0	0.499 999 999 9	0.500 000 000 076 717	1.500 000 003 5	1.500 000 003 671 583
6.0	0.499 999 999 8	0.500 000 000 000 001	1.499 999 999	1.500 000 000 000 001
a	E_2 [8]	E_2 (ours)	E_3 [8]	E_3 (ours)
0.5	44.452 073 828 864	44.452 073 829 740 951	78.996 921 150 976	78.996 921 150 747 460
1.0	11.258 825 780 608	11.258 825 781 482 910	19.899 696 499 3	19.899 696 650 183 008
2.0	3.399 788 240	3.399 788 241 107 422	5.584 639 078 1	5.584 639 079 031 242
3.0	2.541 127 258	2.541 127 259 457 090	3.664 219 644	3.664 219 645 034 898
4.0	2.500 201 179 5	2.500 201 179 960 123	3.501 691 537	3.501 691 538 523 050
5.0	2.500 000 083	2.500 000 084 018 818	3.500 001 22	3.500 001 221 456 053
6.0	2.499 999 998	2.500 000 000 003 671	3.499 999 99	3.500 000 000 080 474
a	E_4 [8]	E_4 (ours)	E_5 [8]	E_5 (ours)
0.5	123.410 710 456 832	123.410 710 456 255 087	177.693 843 822 080	177.693 843 818 557 778
1.0	31.005 254 50	31.005 254 506 369 600	44.577 171 227 1	44.577 171 228 133 505
2.0	8.368 874 427	8.368 874 428 255 031	11.764 982 120 9	11.764 982 122 266 749
3.0	4.954 180 470	4.954 180 470 745 735	6.473 336 615	6.473 336 616 229 402
4.0	4.509 640 989	4.509 640 990 557 537	5.539 421 796	5.539 421 797 077 043
5.0	4.500 012 63	4.500 012 637 250 637	5.500 098 71	5.500 098 717 910 283
6.0	4.500 000 0	4.500 000 001 280 182	5.500 000 1	5.500 000 015 735 293
a	E_{15} [8]	E_{15} (ours)	E_{18} [8]	E_{18} (ours)
0.5	1263.350 931 234	1263.350 931 326 357 881	1781.505 191 022	1781.505 191 087 087 521
1.0	315.993 628 7	315.993 628 787 720 636	445.532 296 7	445.532 296 811 001 395
2.0	79.623 013 2	79.623 013 278 512 904	112.007 801 3	112.007 801 355 885 660
3.0	36.600 930 3	36.600 930 340 754 455	50.991 543 0	50.991 543 053 598 755
4.0	22.471 738 3	22.471 738 352 379 783	30.548 807 3	30.548 807 326 817 998
5.0	17.078 643 2	17.078 643 210 603 116	22.177 796 6	22.177 796 531 345 646
6.0	15.579 546 9	15.579 546 896 354 019	19.008 265 4	19.008 265 304 869 009

2.2. The asymmetric confinement

In order to solve equation (3) with the boundary conditions equation (5) with $a \neq b$, we will use a modified version of a numerical method based on the direct integration of the Schrödinger equation [16]. First, let us take equations (3) and (7) as a system of simultaneous coupled differential equations for ψ and $\dot{\psi} = \partial\psi/\partial\epsilon$. With the following boundary conditions:

$$\psi(a) = 0, \quad \psi'(a) = 1, \quad (15a)$$

and

$$\dot{\psi}(a) = 0, \quad \dot{\psi}'(a) = 0, \quad (15b)$$

where a is the position of the left wall of the box and the prime represents the derivative of the wavefunction with respect to x , taking $\psi'(a) = 1$ is completely arbitrary and does not have

any consequences in determining the eigenvalues. Later on, ψ will be normalized to one. The process of numerical solution proceeds according to the following iteration scheme:

- (i) Choose an initial value of ϵ_i and solve (3) and (7) using the Runge–Kutta method with an adjusted step-size of order 7, 8.
- (ii) Now improve ϵ_i , imposing the second boundary condition $\psi(b, \epsilon) = 0$ using the Newton–Raphson method:

$$\epsilon_{i+1} = \epsilon_i - \frac{\psi(b, \epsilon_i)}{\dot{\psi}(b, \epsilon_i)}. \quad (16)$$

- (iii) Repeat step (ii) until $|\epsilon_{i+1} - \epsilon_i| < \delta$, where δ is equal to a maximum allowed tolerance.

In order to calculate another eigenvalue, we start the process in step (i) with a new guess for ϵ , different enough from the one previously obtained in order to get convergence to a different eigenvalue. For each ϵ obtained, we identify the order of the corresponding state by counting the nodes of ψ . This procedure is particularly useful when we have several eigenvalues lying very close to each other. Once we have calculated the eigenvalue, the same iteration scheme also generates the values of the eigenfunction at a large number of points in $[a, b]$, which can be used to plot or to obtain expectation values of operators, etc. In this manner we can obtain, with a high degree of precision, the eigenvalues of any bounded potential, and even an accurate estimation of the eigenvalues of pseudo-bounded potentials. The energy eigenvalues for the symmetric confinement were calculated using this last method and also with those of section 2.1; we find them to be in complete agreement. In table 2 we compare results for the asymmetrical case with those reported by Vawter [14] and Fernández and Castro [15]. The results of Fernández and Castro [15] become less accurate when the asymmetry increases, as we can see from table 2. In table 3 we show our results for the first six states of the asymmetrically confined harmonic oscillator as a function of the box size. The walls of the box are displaced so that the ratio b/a remains equal to 1.5 in all cases. We can observe that, as the size of the box increases, the eigenvalues approach those of the free harmonic oscillator, as expected.

3. Einstein coefficients

With the energy values and eigenfunctions calculated above we are now able to compute the Einstein B coefficient for induced transitions in the dipolar approximation [26, 27], which is given by

$$B_{mn} = \frac{2\pi}{3\hbar^2} |d_{mn}|^2, \quad (17)$$

where d_{mn} is the dipolar matrix element between the initial and final states n and m , defined as

$$d_{mn} = e \int \psi_m^* x \psi_n dx. \quad (18)$$

Here, e is the electronic charge. In the same approximation the Einstein A coefficient for spontaneous transitions [26, 27] is given by

$$A_{mn} = \frac{2\hbar\omega_{mn}^3}{\pi c^3} B_{mn} = \frac{4\omega_{mn}^3}{3\hbar c^3} |d_{mn}|^2, \quad (19)$$

where $\omega_{mn} = (E_m - E_n)/\hbar$ is the radiation frequency for transitions from the initial state n to the final state m . In general, the dipole matrix elements, and hence the Einstein coefficients, for the confined harmonic oscillator cannot be obtained analytically; however, there are two opposite limiting cases for which this is feasible, although in an approximate way: very small

Table 2. The energy eigenvalues for the ground state and three first excited states of an asymmetrically confined harmonic oscillator, obtained by the present method, and their comparison with those reported by Vawter [14] and Fernández and Castro [15]. The size of the box is $b - a = 2$, $W_n = 2E_n$ (two times the energy) and $d = (b + a)/2$ is the position of the minimum of the harmonic oscillator potential. These quantities were chosen to make a direct comparison with the results of [14] and [15].

d	W_1 [14]	W_1 [15]	W_1 (ours)	W_2 [14]	W_2 [15]	W_2 (ours)
0.00	2.596	2.5969	2.59691966	10.15	10.151	10.151 164 03
0.12	2.610	2.610	2.61034621	10.16	10.167	10.165 829 21
0.24	2.651	2.650	2.65062665	10.21	10.21	10.209 823 96
0.36	2.718	2.717	2.71776341	10.28	10.28	10.283 146 02
0.48	2.812	2.811	2.81176041	10.38	10.39	10.385 791 50
0.60	2.933	2.932	2.93262332	10.52	10.52	10.517 755 19
0.72	3.080	3.080	3.08035913	10.68	10.68	10.679 030 19
0.84	3.255	3.253	3.25497639	10.87	10.87	10.869 608 20
0.96	3.456	3.454	3.45648534	11.09	11.09	11.089 479 78
1.08	3.685	3.681	3.68489748	11.34	11.34	11.338 634 01
1.20	3.940		3.94022544	11.62		11.617 058 38
1.56	4.868		4.86785207	12.63		12.627 852 07
1.92	6.038		6.03830195	13.90		13.901 445 82
2.04	6.482		6.48250177	14.38		14.384 323 67
2.64	9.110		9.10984706	17.23		17.235 295 72
2.88	10.35		10.35084739	18.58		18.579 015 21
3.00	11.01		11.01217154	19.29		19.294 354 69
d	W_3 [14]	W_3 [15]	W_3 (ours)	W_4 [14]	W_4 [15]	W_4 (ours)
0.00	22.52	22.52	22.51765156	39.80	39.80	39.799 393 00
0.12	22.53	22.53	22.53222905	39.81	39.81	39.813 903 15
0.24	22.57	22.58	22.57596148	39.86	39.86	39.857 433 58
0.36	22.65	22.65	22.64884877	39.93	39.93	39.929 984 31
0.48	22.75	22.75	22.75089070	40.03	40.03	40.031 555 28
0.60	22.88	22.87	22.88208716	40.16	40.16	40.162 146 58
0.72	23.04	23.04	23.04243775	40.32	40.32	40.321 758 11
0.84	23.23	23.23	23.23194206	40.51	40.51	40.510 389 77
0.96	23.48	23.43	23.45059983	40.73	40.73	40.728 041 74
1.08	23.70	23.70	23.69841063	40.97	40.97	40.974 714 03
1.20	23.97		23.97537365	41.25		41.250 406 38
1.56	24.98		24.98116971	42.25		42.251 603 78
1.92	26.25		26.24931024	43.51		43.513 981 76
2.04	26.73		26.73031802	43.99		43.992 814 27
2.40	28.35		28.34820879	45.60		45.603 431 23
2.64	29.57		29.57251149	46.82		46.822 273 95
2.88	30.91		30.91336772	48.16		48.157 194 72
3.00	31.63		31.62749854	48.86		48.868 183 46

(free particle in a box) and very large boxes (unbounded harmonic oscillator). For very small boxes ($R \rightarrow 0$) we recover the behaviour of a free particle in a box, being the dipole matrix elements of this system given by

$$|d_{mn}| = \frac{8eR}{\pi^2} \frac{mn}{(m^2 - n^2)^2} |(-1)^{n-m} - 1|. \quad (20)$$

The selection rules in this case establish that the transitions are only possible when $\Delta n = m - n = \text{odd}$, i.e. that the transitions are only allowed between first, third, etc neighbours, in

Table 3. Energy eigenvalues for the ground state and the first five excited states of an asymmetrically confined harmonic oscillator. The walls of the box are located at $x = a$ and b . The length unit is $\sqrt{\hbar/m\omega}$ and the energy unit is $\hbar\omega$.

a	b			
-0.40	0.6	4.956 107 430 509 850	19.779 540 672 522 745	44.457 077 725 690 018
		79.001 923 538 860 975	123.415 712 042 565 422	177.698 844 941 942 980
-0.48	0.72	3.457 577 547 425 262	13.765 858 189 778 583	30.905 677 993 095 790
		54.896 070 185 086 711	85.739 400 962 186 841	123.436 249 789 676 923
-0.64	0.96	1.981 761 162 348 153	7.813 841 869 877 837	17.461 270 959 890 426
		30.958 008 119 516 358	48.308 360 546 469 642	69.513 366 236 762 503
-0.80	1.20	1.317 107 979 433 359	5.095 950 157 502 384	11.279 072 284 988 040
		19.919 849 480 543 796	31.025 356 298 644 810	44.597 243 310 855 157
-1.28	1.92	0.672 627 870 568 576	2.333 779 793 391 920	4.791 367 580 358 017
		8.177 296 991 112 514	12.519 179 402 879 797	17.822 460 577 169 699
-1.60	2.40	0.565 770 255 446 033	1.838 819 613 302 878	3.489 952 647 379 795
		5.674 005 587 304 844	8.455 573 969 729 765	11.849 773 130 644 206
-3.00	4.50	0.500 195 415 964 895	1.503 020 303 422 310	2.519 913 654 479 166
		3.575 115 229 805 945	4.691 640 820 487 011	5.877 825 839 810 553
-4.00	6.00	0.500 000 245 427 974	1.500 007 301 347 236	2.500 100 566 198 534
		3.500 844 396 862 557	4.504 784 483 376 225	5.519 238 717 316 811

agreement with the Laporte rule which states that, in a dipolar transition, the parity of the final state must be different from that of the initial one. On the other hand, for very large boxes ($R \rightarrow \infty$) the free harmonic oscillator behaviour is recovered and the dipole matrix elements are then [26]

$$|d_{mn}| = \begin{cases} e\sqrt{\frac{n+1}{2}} & \text{if } m = n + 1, \\ e\sqrt{\frac{n}{2}}, & \text{if } m = n - 1, \\ 0 & \text{otherwise.} \end{cases} \quad (21)$$

In this case, the selection rules establish that $\Delta n = m - n = \pm 1$, i.e. the transitions are allowed only between first neighbours. In order to calculate the A and B coefficients, equations (17) and (19) respectively, we use the energy eigenvalues and the eigenfunctions obtained in the preceding section to compute the required dipole matrix elements (18). The Einstein A coefficients for the symmetrical and asymmetrical cases are shown in table 4, whereas in table 5 we show the B coefficients for different box sizes. In table 4 we present results for three cases of symmetrical confinement; the others describe asymmetrical confinements. In the symmetrical cases the Laporte rule is satisfied; however, the selection rules for the confined harmonic oscillator are different from those of the free case. For example, the coefficient A_{14} is different from zero in the confined case but vanishes for the unbounded harmonic oscillator. From table 4 we can detect other coefficients different from zero in the confined case and identically zero in the unbounded case. Note that the value of these coefficients diminishes quite quickly when the box size increases. Similar conclusions are obtained for the B coefficients as we can see from table 5. These observations are in agreement with those first obtained using perturbation theory [11], but now, given that our accuracy is much higher, we can study larger parameter regions than those allowed by perturbation theory. In table 4 are also shown the coefficients for the asymmetric confinement as a function of the position of the walls. Note that A_{31} , A_{51} , A_{42} , as well as others, are different from zero in apparent violation of the Laporte rule. The violation of the Laporte rule is only apparent, since in the case of asymmetrical

Table 4. Einstein A_n coefficients for a confined harmonic oscillator. The minimum of the harmonic oscillator potential is at the origin and the walls of the box are located at $x = a$ and $x = b$. The Einstein A_n coefficients are given in units of $4\omega^4 e^2 / 3mc^3$.

(a, b)	$(-0.5, 0.5)$	$(-0.4, 0.6)$	$(-1.0, 1.0)$	$(-0.8, 1.2)$	$(-2.4, 0)$
A_{21}	105.564 593	105.564 876	6.871 390	6.875 814	3.688 705
A_{31}	0.000 000	0.000 700	0.000 000	0.010 372	0.462 733
A_{41}	83.903 350	83.903 591	4.954 881	4.958 535	2.413 204
A_{51}	0.000 000	0.000 567	0.000 000	0.008 330	0.371 075
A_{61}	80.919 567	80.919 784	4.790 460	4.793 762	2.329 297
A_{32}	568.761 161	568.760 679	35.808 245	35.801 382	17.139 700
A_{42}	0.000 000	0.000 264	0.000 000	0.004 449	0.243 432
A_{52}	375.239 280	375.238 936	22.761 715	22.756 934	10.415 362
A_{62}	0.000 000	0.000 176	0.000 000	0.002 972	0.163 441
A_{43}	1624.673 715	1624.673 378	101.931 787	101.926 398	49.093 306
A_{53}	0.000 0000	0.000 162	0.000 000	0.002 681	0.143 890
A_{63}	946.526 396	946.526 195	58.261 449	58.258 266	27.440 096
A_{54}	3509.767 604	3509.767 353	219.895 853	219.891 805	106.125 360
A_{64}	0.000 000	0.000 119	0.000 000	0.001 936	0.102 419
A_{65}	6460.834 064	6460.833 865	404.482 654	404.479 443	195.267 172
(a, b)	$(-2.0, 2.0)$	$(-1.6, 2.4)$	$(-4.0, 0.0)$	$(-4.0, 0.2)$	$(-4.4, -0.2)$
A_{21}	0.743 447	0.787 811	1.702 856	1.532 642	1.876 490
A_{31}	0.000 000	0.047 738	0.702 656	0.590 925	0.794 185
A_{41}	0.123 109	0.145 751	0.590 267	0.479 277	0.624 405
A_{51}	0.000 000	0.035 588	0.560 778	0.455 312	0.594 725
A_{61}	0.126 741	0.147 708	0.576 727	0.466 177	0.604 616
A_{32}	2.585 014	2.597 996	3.363 705	3.057 412	3.472 387
A_{42}	0.000 000	0.083 379	1.257 589	1.113 526	1.393 628
A_{52}	0.857 156	0.867 001	1.243 963	1.029 093	1.196 147
A_{62}	0.000 000	0.054 965	0.901 446	0.796 927	1.012 269
A_{43}	6.744 958	6.688 467	6.302 474	5.431 427	5.651 035
A_{53}	0.000 000	0.060 891	1.371 624	1.335 117	1.788 117
A_{63}	2.766 779	2.739 290	2.547 740	2.033 995	2.122 980
A_{54}	14.230 077	14.162 383	12.888 061	10.599 708	10.328 312
A_{64}	0.000 000	0.040 198	1.036 044	1.075 700	1.566 828
A_{65}	25.910 391	25.853 028	24.523 389	20.053 596	19.491 765

confinement the oscillator states do not have well defined parities. This type of confinement leads to the appearance of transitions that were forbidden before, thus increasing the number of nonzero Einstein coefficients. In figure 1 we show the Einstein coefficients A_{24} and B_{24} as a function of the box size and of the asymmetry parameter d . These coefficients are identically equal to zero for $d = 0$, in agreement with the Laporte rule. This fact is clearly observed from figures 1(a) and (b). For $d \neq 0$ these coefficients can be small but they are not necessarily zero, as we can see from figure 1(a) and (b) and from tables 4 and 5. It is easy to observe increasing values of A_{24} and B_{24} as R and d increase. This fact can also be appreciated from tables 4 and 5. In this way we see that the complexity of the emission and the absorption spectra is considerably increased by the confinement to the inside of a quantum box.

4. Conclusions

We have studied in this work the energy spectrum and the Einstein A and B coefficients for a symmetrical and asymmetrical confined one-dimensional harmonic oscillator. We have

Table 5. Einstein B_n coefficients for a confined harmonic oscillator. The minimum of the harmonic oscillator potential is at the origin and the walls of the box are located at $x = a$ and b . The B_n coefficients are in units of $2\pi e^2/3m\hbar\omega$.

(a, b)	(-0.5, 0.5)	(-1.0, 1.0)	(-2.0, 2.0)	(-0.4, 0.6)	(-0.8, 1.2)
B_{21}	0.032 409 652	0.127 515 080	0.402 105 072	0.032 409 552	0.127 423 014
B_{31}	0.000 000 000	0.000 000 000	0.000 000 000	0.000 000 011	0.000 010 491
B_{41}	0.000 206 670	0.000 769 853	0.000 957 513	0.000 206 670	0.000 770 233
B_{51}	0.000 000 000	0.000 000 000	0.000 000 000	0.000 000 000	0.000 000 317
B_{61}	0.000 015 698	0.000 059 095	0.000 089 550	0.000 015 698	0.000 059 130
B_{32}	0.037 846 381	0.151 472 551	0.591 469 298	0.037 846 360	0.151 452 455
B_{42}	0.000 000 000	0.000 000 000	0.000 000 000	0.000 000 001	0.000 001 366
B_{52}	0.000 337 111	0.001 305 611	0.002 975 962	0.000 337 111	0.001 305 377
B_{62}	0.000 000 000	0.000 000 000	0.000 000 000	0.000 000 000	0.000 000 048
B_{43}	0.039 410 897	0.157 992 735	0.646 716 479	0.039 410 894	0.157 989 512
B_{53}	0.000 000 000	0.000 000 000	0.000 000 000	0.000 000 000	0.000 000 348
B_{63}	0.000 400 139	0.001 575 182	0.004 726 574	0.000 400 139	0.001 575 121
B_{54}	0.040 061 285	0.160 544 668	0.659 309 650	0.040 061 284	0.160 543 932
B_{64}	0.000 000 000	0.000 000 000	0.000 000 000	0.000 000 000	0.000 000 128
B_{65}	0.040 391 860	0.161 799 190	0.661 499 650	0.040 391 860	0.161 798 968
(a, b)	(-2.4, 0.0)	(-1.6, 2.4)	(-4.0, 0.0)	(-4.0, 0.2)	(-4.4, -0.2)
B_{21}	0.168 572 771	0.381 844 581	0.212 322 553	0.227 542 683	0.198 773 948
B_{31}	0.001 293 484	0.001 909 225	0.010 660 805	0.010 556 679	0.010 656 951
B_{41}	0.001 074 267	0.001 093 450	0.002 367 762	0.002 306 881	0.002 398 302
B_{51}	0.000 041 195	0.001 093 450	0.000 760 673	0.000 763 894	0.000 848 448
B_{61}	0.000 084 313	0.000 102 805	0.000 303 600	0.000 310 594	0.000 358 872
B_{32}	0.215 294 552	0.577 154 868	0.397 537 319	0.420 831 386	0.377 783 869
B_{42}	0.000 222 798	0.001 478 083	0.015 906 082	0.016 960 459	0.017 876 230
B_{52}	0.001 783 021	0.002 992 848	0.003 577 438	0.003 700 623	0.003 855 609
B_{62}	0.000 007 916	0.000 054 785	0.000 805 292	0.000 911 837	0.001 080 269
B_{43}	0.227 536 552	0.642 003 083	0.550 174 374	0.588 681 843	0.547 565 541
B_{53}	0.000 055 863	0.000 497 320	0.011 010 854	0.013 802 732	0.017 501 833
B_{63}	0.002 217 075	0.004 688 644	0.004 383 409	0.004 589 608	0.004 666 786
B_{54}	0.231 552 924	0.658 062 469	0.626 518 074	0.684 090 232	0.662 848 459
B_{64}	0.000 020 362	0.000 170 663	0.004 584 373	0.006 372 028	0.009 347 504
B_{65}	0.233 335 958	0.661 149 168	0.651 628 038	0.718 218 878	0.710 491 753

used methods that produce high-precision energy eigenvalues and eigenfunctions. The energy eigenvalues that we obtained for the confined oscillator are compared with those reported in the literature [8, 13–15], showing that some energy values considered as exact ones are only good approximations, and that the values calculated here are far more accurate. The values obtained by the methods described in this paper can then be used as a reference for future calculations.

For a confined oscillator we found that the selection rules of the unbounded oscillator are not satisfied. In the symmetrical confinement the states of the oscillator have definite parity and the Laporte rule is satisfied. However, coefficients like A_{61} are different from zero, while this coefficient is zero for the unbounded harmonic oscillator. In the asymmetrical confinement, the wavefunctions do not have definite parity, and the Laporte rule does not apply. The Einstein A and B coefficients for this problem are, in general, different from zero, showing that this type of confinement introduces a complexity in the emission or absorption spectra.

Although this is a very simple model, some of the qualitative features will be preserved when more complex systems are considered, so we can expect in general an increase in the

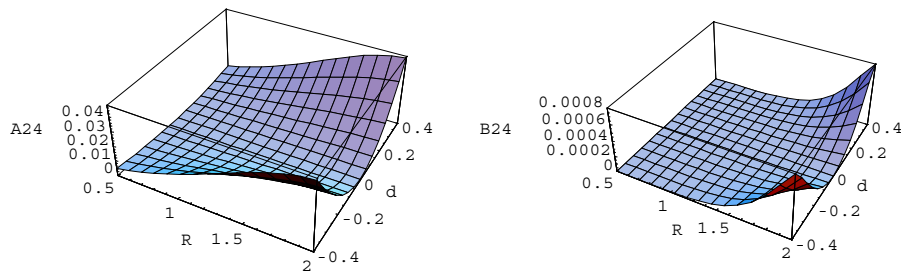


Figure 1. The Einstein coefficients A_{24} and B_{24} as a function of the box size and the asymmetry parameter d . A_{24} is given in units of $4\omega^4 e^2 / 3mc^3$, whereas B_{24} is in units of $2\pi e^2 / 3m\hbar\omega$. These coefficients are identical to zero for symmetric confinement $d = 0$, and they are small for small boxes, but they grow as a function of R and d .

(This figure is in colour only in the electronic version)

number of nonzero Einstein coefficients in a system, when we submit it to confinement. This would be of great technological interest, since devices emitting or absorbing radiation in selected frequencies could be produced and the frequencies involved would be regulated by adjusting the size of the system confinement.

We must mention that the way in which we introduced the spatial confinement is not the only one: two different approaches were developed by other authors [28, 29], and in some limiting case their confinement is equivalent to that used here.

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