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Quantum symmetrical quadratic potential in a box

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Abstract. The quantum mechanical problem of a repulsive quadratic potential in a box is solved by an algebraic and numerical computer technique. The energy eigenvalues are tabulated for various box sizes and the lowest energy level is tabulated as a function of the quadratic potential strength, where the potential varies from strongly attractive through zero to strongly repulsive. Tunnelling and level pairing are seen to occur.

Besides being of obvious theoretical interest, the quantum system of a particle moving in a bounded quadratic potential appears in several physical situations. For instance, a critical point of infinite type (Benguigui 1977) can be described by means of a transition from an attractive to a repulsive quadratic potential in an infinite well.

The solution for the boxed attractive quadratic potential was found recently by Consortini and Frieden (1976) by means of a numerical procedure. In what follows, the solution for the repulsive quadratic potential is found in a similar way. Following this, the lowest energy level is calculated as a function of the strength of the quadratic potential, where the potential varies from strongly attractive through zero to strongly repulsive.

Let us consider a particle of mass m confined within two infinitely repulsive potentials separated by a distance $2x_0$ and acted upon by a quadratic potential $V(x)=-\frac{1}{2}kx^2$, where k is obviously a constant. For simplicity we work in one dimension and consider only a symmetrical potential (see figure 1). The Schrödinger equation for this system is given by

$$-(\hbar^2/2m)\psi''(x)-\tfrac{1}{2}|k|x^2\psi(x)=E\psi(x) \tag{1}$$

for $-x_0<x<x_0$ and zero elsewhere. Defining the dimensionless quantities

$$t=\alpha x, \qquad a=-E/\beta \tag{2}$$

where

$$\alpha^4=4|k|m/\hbar^2, \qquad \beta=\hbar(|k|/m)^{1/2}\equiv\hbar\omega$$

transforms equation (1) into the standard parabolic cylinder function

$$(\mathrm{d}^2y(t)/\mathrm{d}t^2)+(\tfrac{1}{4}t^2-a)y(t)=0. \tag{3}$$

This has a solution (Abramowitz and Stegun 1964) of the form

$$y(t)=Ay_1(t)+By_2(t) \tag{4}$$

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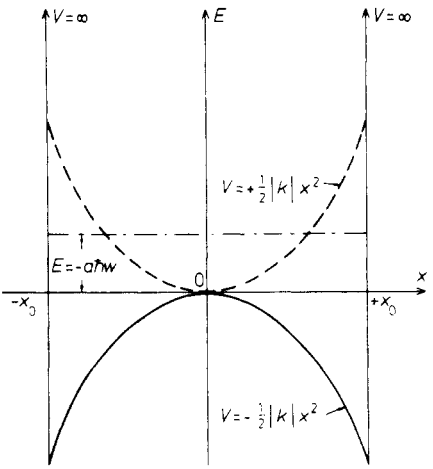

Figure 1. Auadratic potentials in a box. Note that E and a have opposite signs.

where

$$y_1(t) = 1 + \sum_{n(\text{even})=2}^{\infty} c_n t^n / n! \tag{4a}$$

$$y_2(t) = t + \sum_{n(\text{odd})=3}^{\infty} c_n t^n / n! \tag{4b}$$

are even and odd functions of t respectively. The coefficients c_n are defined by

$$c_n = a c_{n-2} - \tfrac{1}{4}(n-2)(n-3)c_{n-4} \qquad \begin{cases} c_0 = 1 \\ c_1 = 1 \end{cases} \tag{4c}$$

where it should be remembered that the a are the dimensionless energy eigenvalues that are required. From its definition (2), and from figure 1, it is clear that a will be negative for energy levels above the peak of the quadratic potential and positive below.

The boundary conditions are given by

$$\psi(x_0) = \psi(-x_0) = 0 \tag{5}$$

which transforms to

$$y(t_0) = y(-t_0) = 0 \qquad \text{for } t_0 = \alpha x_0. \tag{6}$$

From equation (4) these are obviously satisfied by

$$y_1(t_0) = 0, \qquad B = 0 \tag{7}$$

or

$$y_2(t_0) = 0, \qquad A = 0.$$

This means that the even and odd solutions (4*a*) and (4*b*) can be treated separately. Using the LISP 1·5 based algebraic manipulation program REDUCE 2 (Hearn 1973), equations (4*a*) and (4*b*) were each evaluated and expressed as a polynomial of order 49 or less in a.

By the boundary conditions (7) these polynomials are equal to zero at the box walls and hence, for each half-well width t_0, solving for the roots of the polynomials will give

the eigenvalues a. This was done using standard FORTRAN IV techniques. Since standard library programs were used, the order of the polynomials had to be adjusted for each value of t_0 to be the maximum possible without generating numbers smaller than those the computor, an IBM 370/168, was able to handle. This limited the number of accurate eigenvalues for each value of t_0 to about $N/2$, where N was the order of the polynomial in a.

IBM double precision, i.e. 15–16 significant figures, was used throughout and the accuracy of the results was established by two means. Firstly the algorithm chosen for calculating the roots of the polynomials calculated the complex roots, and hence any eigenvalue with a non-negligible imaginary part was discarded as being due to the finite order of the polynomial. Secondly, and most importantly, for each value of t_0 the calculation was performed twice, the second time decreasing the order of the polynomial by one. Then, for each eigenvalue, only significant figures which remained unchanged by the decrease in order were known to be correct. This in general gave an accuracy of better than 13 significant figures for the lower eigenvalues. However, for the sake of compactness, generally only 10 or less figures are quoted. These are tabulated in table 1. The half-well width t_0 is expressed as multiples of $\sqrt{2}$ to facilitate

Table 1. Energy levels a_n as a function of t_0.

t_0	$\frac{1}{4}\sqrt{2}$	$\sqrt{2}$	$2\sqrt{2}$	$\frac{5}{2}\sqrt{2}$
	−19·735 124 56	−1·167 756 672	−0·002 263 391 345	0·422 041 453 6
	−78·948 001 55	−4·792 906 634	−0·631 464 302 2	0·238 320 840 9
	−177·643 166 2	−10·948 019 88	−2·168 354 462	−0·898 556 498 7
	−315·817 320 0	−19·579 030 86	−4·304 526 926	−2·202 110 435
	−493·470 056 7	−30·680 027 47	−7·068 585 568	−3·951 576 436
	−710·601 276 1	−44·249 467 00	−10·454 316 14	−6·106 763 451
	−967·21	−60·286 805 98	−14·459 431 81	−8·662 548 656
	−1263	−78·791 813 80	−19·082 846 13	−11·616 438 56
		−99·764 379 20	−24·323 993 51	−14·976 153 26
		−123·204 443 20	−30·182 557 8	−18·713 974 51
		−149·111 972	−36·658 351 8	−22·856 473 30
		−177·487	−43·751 259 2	−27·394 381
		−208·3	−51·461 204 8	−32·327 52
			−59·788 138	−37·655 78
t_0	$\frac{1}{2}\sqrt{2}$	$\frac{3}{2}\sqrt{2}$	−68·732 03	−43·379 1
			−78·293	−49·497 3
	−4·918 456 570	−0·394 174 138 9	−88	−56·01
	−19·703 865 99	−1·868 810 530		−62·9
	−44·374 369 46	−4·586 822 479		
	−78·916 754 11	−8·414 065 073		
	−123·329 403 5	−13·343 368 82		
	−177·611 917 7	−19·371 676 58		
	−241·764 159 3	−26·497 796 91		
	−315·786 070 9	−34·721 196 20		
	−399·677 6	−44·041 608 35		
	−493·44	−54·458 889 19		
	−597	−65·972 955 28		
		−78·583 755 6		
		−92·291 257		
		−107·095 4		
		−123·00		

Table 1—(*continued*)

t_0	$3\sqrt{2}$	$\frac{7}{2}\sqrt{2}$	$4\sqrt{2}$	$5\sqrt{2}$
	1·170 473 176	2·297 879 314	3·725 613 244	7·410 033 475 2
	1·150 858 052	2·297 205 136	3·725 604 475	7·410 033 475 1
	−0·200 106 508	0·319 978 301 4	1·182 241 966	4·100 478 458
	−0·883 199 160	0·122 202 076 4	1·166 966 529	4·100 476 265
	−2·066 066 919	−0·815 555 932	−0·074 039 057 53	1·803 959 653
	−3·534 573 368	−1·806 095 484	−0·546 767 452 0	1·801 833 364
	−5·292 329 667	−3·061 287 327	−1·465 416 687	0·315 260 579
	−7·332 137 157	−4·535 361 786	−2·540 498 012	0·148 343 961
	−9·650 876 187	−6·221 751 383	−3·797 839 981	−0·651 960 566
	−12·246 847 96	−8·116 430 729	−5·223 984 98	−1·400 891 042
	−15·119 052 66	−10·217 127 09	−6·813 958 59	−2·333 055 76
	−18·266 867 2	−12·522 449 19	−8·564 768 02	−3·387 419 7
	−21·689 886	−15·031 499 8	−10·474 530 8	−4·558 579 8
	−25·387 835	−17·743 677	−12·542 000	−5·841 031
	−29·360 52	−20·658 56	−14·766 320	−7·231 459
	−33·607 82	−23·775 86	−17·146 88	−8·727 62
	−38·130	−27·095	−19·683 23	−10·328 0
	−42·926	−30·617	−22·375	−12·031 3
	−48·00	−34·34	−25·222	−13·837
	−53·35	−38·3	−28·2	−15·74
	−59	−42·4	−31·4	−17·75
			−34·7	−19·9
				−22·2
				−24

comparison with the results for a positive quadratic potential (Consortini and Frieden 1976).†

From these results it can be seen that as t_0 becomes small the eigenvalues approach those of an infinite square well, namely

$$a_n = -\frac{\pi^2 n^2}{4t_0^2} \qquad n = 1, 2, 3 \ldots . \tag{8}$$

Even for moderate t_0 this agreement exists for the highest energy levels. Of course this is to be expected, since as the well narrows, or the particle energy is very large, the quadratic potential appears to the particle as an approximately flat potential.

As t_0 increases, the particle sees the well split into two wells separated by the quadratic potential, and it would be expected that because of the symmetry of the situation the probability distributions would be equal in each well. This is in fact what happens. For t_0 such that the particle has a narrow potential between the two wells, tunnelling occurs, while for greater t_0, where the potential appears very wide to the lower energy levels, the penetration factor becomes very small. At this stage the eigenvalues become very closely paired. The separation between pair members is in agreement with a WKB calculation (Landau and Lifshitz 1975), which gives the

† Graphical plots of the first two eigenfunctions for each t_0 were made. However, due to lack of space, they were not included but will be made available privately.

separation between these members by†

$$a_n - a_{n+1} \sim \exp(-a_n \pi) \tag{9}$$

for $a_n - a_{n+1} \ll 1$.

To calculate the lowest energy level as a function of quadratic potential strength we first define a dimensionless energy and potential energy by

$$\epsilon = E/\sigma = -2at_0^2\sigma$$
$$\nu = (\gamma/2)|k|x_0^2/\sigma = (\gamma/2)t_0^4 \tag{10}$$

where

$$\sigma = \hbar^2/4mx_0^2, \qquad \gamma = k/|k|.$$

Then for each value of ν, t_0 is given by equation (10) and the above computer program used to calculate a and hence ϵ.

For attractive potentials, that is $\gamma = +1$, the same procedure is used except that equation (4*c*) must be replaced by

$$c_n = a_{n-2} + \tfrac{1}{4}(n-2)(n-3)c_{n-4} \qquad \begin{cases} c_0 = 1 \\ c_1 = 1 \end{cases} \tag{11}$$

The results of these calculations are listed in table 2.

Table 2. Lowest energy level ϵ as a function of ν.

ν	ϵ	ν	ϵ	ν	ϵ	ν	ϵ
390	27·928 671 52	140	16·756 841 55	−110	−20·881 612 95	−360	−146·591 714 8
380	27·568 323 65	130	16·154 744 10	−120	−24·596 641 50	−370	−152·410 278 9
370	27·203 208 08	120	15·530 865 06	−130	−28·508 289 21	−380	−158·265 131 9
360	26·833 131 24	110	14·882 937 743	−140	−32·597 911 62	−390	−164·154 993 2
350	26·457 886 23	100	14·208 327 84	−150	−36·847 870 62	−400	−170·078 663 3
340	26·077 251 49	90	13·503 961 00	−160	−41·242 143 18	−410	−176·035 016 1
330	25·690 989 33	80	12·766 226 39	−170	−45·766 544 33	−420	−182·022 992 8
320	25·298 844 30	70	11·990 863 17	−180	−50·408 709 23	−430	−188·041 596 1
310	24·900 541 28	60	11·172 818 81	−190	−55·157 947 42	−440	−194·089 885 1
300	24·495 783 36	50	10·306 076 67	−200	−60·005 044 11	−450	−200·166 971 4
290	24·084 249 42	40	9·383 448 232	−210	−64·942 052 23	−460	−206·272 015 0
280	23·665 591 32	30	8·396 258 511	−220	−69·962 097 85	−470	−212·404 220 6
270	23·239 430 72	20	7·334 418 403	−230	−75·059 208 34	−480	−218·562 835 4
260	22·805 355 42	10	6·185 428 944	−240	−80·228 165 83	−490	−224·747 145 6
250	22·362 915 07	0	4·934 802 201	−250	−85·464 384 56	−500	−230·956 474 5
240	21·911 616 30	−10	3·565 514 537	−260	−90·763 809 51	−510	−237·190 180 0
230	21·450 916 92	−20	2·058 070 649	−270	−96·122 833 01	−520	−243·447 652 8
220	20·980 219 24	−30	0·390 841 943 0	−280	−101·538 226 4	−530	−249·728 314 4
210	20·498 862 20	−40	−1·459 075 413	−290	−107·007 083 8	−540	−256·031 615 3
200	20·006 112 08	−50	−3·514 356 233	−300	−112·526 776 2	−550	−262·357 033 4
190	19·501 151 47	−60	−5·795 337 978	−310	−118·094 912 8	−560	−268·704 072 2
180	18·983 066 23	−70	−8·317 634 706	−320	−123·709 310 1	−570	−275·072 258 9
170	18·450 829 86	−80	−11·090 077 36	−330	−129·367 965 0	−580	−281·461 143 1
160	17·903 284 73	−90	−14·113 640 52	−340	−135·069 033 0	−590	−287·870 294 7
150	17·339 119 46	−100	−17·381 720 13	−350	−140·810 809 7	−600	−294·229 301 6

† Of course, the WKB method cannot be used to give the normalisation constants for the lowest levels; rather an exact calculation would be needed. However, the exponential term is the same in any case.

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