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1980 J. Phys. A: Math. Gen. 13 3585

(http://iopscience.iop.org/0305-4470/13/12/008)

J. Phys. A: Math. Gen. **13** (1980) 3585–3598. Printed in Great Britain

# Perturbative, asymptotic and Padé-approximant solutions for harmonic and inverted oscillators in a box†

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Received 5 March 1980, in final form 30 May 1980

**Abstract.** The energy levels of boxed-in harmonic and inverted oscillators are constructed from the perturbative and asymptotic solutions that are valid in the limits of small and large sizes, respectively.

In order to obtain expressions for the energy levels which are valid for boxes of any size, we use Padé approximants constructed as interpolations between the perturbative and asymptotic solutions. Special attention is paid to the lowest levels.

The accuracy and range of validity of each type of solution are illustrated by comparing them with the exact solution which is obtained by constructing and diagonalising the matrix of the Hamiltonian of the system in the basis of eigenfunctions of the free particle in a box.

## 1. Introduction

The quantum-mechanical problem of the symmetrical quadratic potential in a box was solved, for the attractive case, by Consortini and Frieden (1976), while the repulsive case was considered more recently by Rotbart (1978). Their method of solution consists in using numerical computer techniques.

We have investigated the same problem with the objective of finding approximate analytic expressions for the energy levels. For relatively small sizes the perturbative solutions are good, while for relatively large sizes the asymptotic solutions are valid. In order to find closed expressions for the energy levels that are valid for boxes of any size, we use Padé approximants constructed as interpolations between the perturbative and asymptotic solutions, which, as already mentioned, are valid for small and large sizes, respectively.

In order to establish clearly the connections between the approximate solutions and the exact ones, we start from the Schrödinger equations

$$H\psi(\xi)=\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\pm\tfrac{1}{2}\xi^2\right)\psi(\xi)=\epsilon\psi(\xi) \tag{1}$$

where the plus and minus signs correspond to the attractive and repulsive cases, respectively. The energy is measured in units of $\hbar\omega$ and the unit of distance is

† Work supported by FINEP, Rio de Janeiro, under contract 522/CT.
‡ On leave of absence from Instituto de Física, University of México, with financial support of FAPESP, São Paulo, Brasil.

0305-4470/80/123585 + 14$01.50  

$b=(m\omega/\hbar)^{1/2}$, in terms of the mass $m$ and frequency $\omega$ of the system. For a symmetrical box of size $2R$, the boundary conditions on the wavefunctions are

$$\psi(\xi=-R/b)=\psi(\xi=R/b)=0. \tag{2}$$

The symmetry of the potential gives the wavefunctions a definite parity, and allows us to work in the half interval $0\leqslant\xi\leqslant R/b$, with the additional boundary conditions

$$\psi'_+(\xi=0)=0 \tag{3a}$$

$$\psi_-(\xi=0)=0 \tag{3b}$$

for positive and negative parity states, respectively.

The corresponding exact solutions can be written in terms of the Kummer function $M(a, b, z)$ as (Abramowitz and Stegun 1965)

$$\psi^{\mathrm{a}}_+(\xi)=A\,\mathrm{e}^{-\xi^2/2}M(\tfrac{1}{4}(1-2\epsilon),\tfrac{1}{2},\xi^2) \tag{4a}$$

$$\psi^{\mathrm{a}}_-(\xi)=B\,\mathrm{e}^{-\xi^2/2}\xi M(\tfrac{1}{4}(3-2\epsilon),\tfrac{3}{2},\xi^2) \tag{4b}$$

for the attractive case and

$$\psi^{\mathrm{r}}_+(\xi)=C\,\mathrm{e}^{-\mathrm{i}\xi^2/2}M(\tfrac{1}{4}(1+2\mathrm{i}\epsilon),\tfrac{1}{2},\mathrm{i}\xi^2) \tag{5a}$$

$$\psi^{\mathrm{r}}_-(\xi)=D\,\mathrm{e}^{-\mathrm{i}\xi^2/2}\xi M(\tfrac{1}{4}(3+2\mathrm{i}\epsilon),\tfrac{3}{2},i\xi^2) \tag{5b}$$

for the repulsive case.

It is obvious that the boundary conditions related to the parity symmetry (equations ($3a$) and $3(b)$) are satisfied by these functions. On the other hand, the boundary condition related to the box, (equation (2)) will determine the energy eigenvalues.

Another alternative form of an exact formulation of the problem consists in constructing and diagonalising the matrix of the Hamiltonian of the system in the basis of the free-particle eigenfunctions in a box, namely

$$\phi_n^{(+)}(\xi)=\sqrt{b/R}\cos[(2n+1)\pi b\xi/2R] \qquad n=0,1,2,\ldots \tag{6a}$$

$$\phi_n^{(-)}(\xi)=\sqrt{b/R}\sin[(2n)\pi b\xi/2R] \qquad n=1,2,\ldots, \tag{6b}$$

which also satisfy the boundary conditions, equations (2), ($3a$) and ($3b$) in an obvious way. We have performed the numerical solution of this formulation by taking a finite number of basis functions and diagonalising the corresponding submatrix of the Hamiltonian

$$\langle N|H|N'\rangle=\left[\frac{N^2\pi^2}{8}\left(\frac{b}{R}\right)^2\pm\left(\frac{1}{6}-\frac{1}{N^2\pi^2}\right)\left(\frac{R}{b}\right)^2\right]\delta_{N'N}$$
$$\pm(-1)^{(N-N')/2}(1-\delta_{N'N})\frac{16N'N}{\pi^2(N^2-N'^2)^2}\left(\frac{R}{b}\right)^2 \tag{7}$$

where $N$ and $N'$ are both even ($=2n$) or both odd ($=2n+1$). By changing the dimension of the basis sub-space, we can be sure of the convergence and accuracy of the energy eigenvalues for a box of a given size.

In § 2, we develop first the perturbative solutions valid for boxes of small size using the same basis of equations ($6a$) and ($6b$). Next we construct the asymptotic solutions valid for boxes of large size. For the attractive case, the asymptotic form of Kummer's function in equations ($4a$) and ($4b$) with the boundary condition equation (2) leads to the corresponding expression for the energy levels for such boxes. For the repulsive case, the same method applied to equations (5*a*) and (5*b*) shows a slow numerical convergence and does not lead to a simple closed expression for the energy levels. Alternatively, in § 3, we show that for large boxes, in the repulsive case, the linear approximation for the potential is a good starting point for a perturbative asymptotic expansion (large $R$). In § 4 we construct the Padé approximants for the energy levels for boxes of any size by requiring that they tend to the expressions of the small and large size limits.

All these developments are performed especially for the two lowest levels. Of course, they can also be performed for higher levels in which case the convergence of the procedure is slower.

In § 5 we present the diagonalisation values obtained from equation (7), which, according to the accuracy of our calculation, can be called exact.

In § 6 we give the numerical results obtained from the perturbative, asymptotic and Padé approximants and compare them with the exact results of § 5.

## 2. The perturbative and asymptotic expressions for the energy eigenvalues

Taking as unperturbed wavefunctions the expressions given in equations (6*a*) and (6*b*), it is easy to see that each perturbative order of the energy expansion gives an extra $R^4$ (from now on, $R$ is measured in units of $b$). This means that the perturbation expansion has $R^4$ as its perturbative parameter. For instance, the two lower levels, when calculated with the help of the Rayleigh–Schrödinger expansion up to third order, are given by

$$E_{\pm}^{(+)}(R) = 1{\cdot}233\,705\,5\, R^{-2} \pm 0{\cdot}065\,345\,483\, R^2 - 5{\cdot}922\,557\,6\times 10^{-4}\, R^6 \pm 1{\cdot}611\,389\,5\times 10^{-5}\, R^{10} \tag{8}$$

$$E_{\pm}^{(-)}(R) = 4{\cdot}934\,802\,201\, R^{-2} \pm 0{\cdot}141\,336\,308\, R^2 - 1{\cdot}380\,406\,4\times 10^{-4}\, R^6 \pm 5{\cdot}450\,258\,2\times 10^{-7}\, R^{10}. \tag{9}$$

The lower $\pm$ signs correspond to the two signs which appear in equation (1), while the upper signs correspond to the two parity states.

The expressions (8) and (9) are valid for sufficiently small $R$.

Let us now consider the case of large $R$ for the attractive case. By taking the asymptotic expansion of the Kummer functions (Abramowitz and Stegun 1965) which appear in equations (4*a*) and 4(*b*) and using the boundary conditions equations (2), it is not difficult to see that the energy eigenvalues for large $R$ are given by

$$E_{+}^{(+)} = 2k + \tfrac{1}{2} + 2\,\mathrm{e}^{-R^2}\, R^{2(2k+\frac{1}{2})}/\Gamma(k+\tfrac{1}{2})k! \tag{10}$$

$$E_{+}^{(-)} = 2k + \tfrac{3}{2} + 2\,\mathrm{e}^{-R^2}\, R^{2(2k+\frac{3}{2})}/\Gamma(k+\tfrac{3}{2})k! \tag{11}$$

with $k = 0, 1, 2, \ldots$.

These two last expressions explain why, for the attractive case and for values of $R$ which are not too large, the energy eigenvalues tend to $2k+\frac{1}{2}$ and $2k+\frac{3}{2}$ rather rapidly.

For the repulsive case, as we have already mentioned, the same method applied to equations (5*a*) and (5*b*) with the boundary condition equation (2) shows a slow numerical convergence and does not lead to a simple closed expression for the energy levels. We will see in the next section that in this case the linear approximation for the potential is a good starting point.

## 3. The asymptotic expansion for the energy eigenvalues in the repulsive case

Let us rewrite equation (1) and the boundary condition equation (2) in terms of the new variable $\zeta = \xi + R$:

$$\left(-\frac{1}{2}\frac{d^2}{d\zeta^2} + R\zeta - \tfrac{1}{2}\zeta^2\right)\psi(\zeta) = (\epsilon + \tfrac{1}{2}R^2)\psi(\zeta) \tag{12}$$

and

$$\psi(\zeta = 0) = 0. \tag{13}$$

The eigensolutions of

$$\left(-\frac{1}{2}\frac{d^2}{d\zeta^2} + R\zeta\right)\phi(\zeta) = \epsilon^0\phi(\zeta) \tag{14}$$

are

$$\phi_s(\zeta) = N_s \operatorname{Ai}(\zeta/a - \epsilon_s^0/Ra) \tag{15}$$

with

$$a^3 = 1/2R \tag{16}$$

and

$$\epsilon_s^0 = 2^{-1/3}R^{2/3}a_s \tag{17}$$

and Ai is the Airy function whose zeros $a_s$ are given by Abramowitz and Stegun (1965). In equation (15), $N_s$ is a normalisation factor.

Considering the term $-\frac{1}{2}\zeta^2$ in equation (12) as a 'perturbation', the first-order energy correction is given by the matrix element

$$\langle\phi_s|\zeta^2|\phi_s\rangle = \int_0^\infty \phi_s^*\zeta^2\phi_s\,d\zeta.$$

The expression for this can be found in Castilho-Alcarás and Leal-Ferreira (1975) and it gives the contribution

$$\Delta\epsilon_s^{(1)} = -4(2R)^{-2/3}a_s^2/15. \tag{18}$$

Now, for the second-order correction

$$\Delta\epsilon_s^{(2)} = -\tfrac{1}{4}\sum_{m\neq s}\frac{\langle\phi_s|\zeta^2|\phi_m\rangle\langle\phi_m|\zeta^2|\phi_s\rangle}{\epsilon_m^0 - \epsilon_s^0},$$

which, by using the matrix elements given in the appendix, can be written as

$$\Delta\epsilon_s^{(2)} = -72R^{-2}\sum_{m\neq s}(a_s - a_m)^{-9}. \tag{19}$$

therefore, up to second order, equations (17), (18) and (19) give the following expansion for $\epsilon$:

$$\epsilon_s = -\tfrac{1}{2}R^2 - 2^{-1/3}R^{2/3}a_s - \tfrac{4}{15}a_s^2(2R)^{-2/3} - 72R^{-2}\sum_{m\neq s}(a_s - a_m)^{-9}. \tag{20}$$

Strictly speaking, the matrix elements we should calculate are of the form $\int_0^{2R} \phi_s^* \zeta^2 \phi_{s'} \,\mathrm{d}\zeta$. But for large $R$, $\phi_s$ decays exponentially and therefore the expansion given in equation (20) is valid up to terms which decay exponentially for large $R$.

Let us recall that in this approximation the even and odd states are degenerate.

## 4. Padé approximants

With the expressions (8) and (9) valid for small $R$ and expressions (10), (11) as well as (20) valid for large $R$, we can construct the two-point Padé approximants (Baker 1975) which interpolate the large and small box sizes.

For the harmonic potential we have first considered the one-point Padé approximants [2/5] and [3/4] constructed for $R^2(E_+^{(+)}(R)-\frac{1}{2})$ and $R^2(E_+^{(-)}(R)-\frac{3}{2})$, where for small $R$ we use for $E_+^{(+)}$ and $E_+^{(-)}$ the expansions given by equations (8) and (9). These functions go to zero for $R\to\infty$ and this determines the choice of one-point Padé approximants with the numerator of smaller degree than the denominator.

In this way, we obtain approximate expressions for $E_+^{(+)}$ and $E_+^{(-)}$ valid for any value of $R$. For instance, with the help of the [3/4] Padé approximants, we have

$$E_{+[3/4]}^{(+)}(R) = R^{-2}[3/4]_+^{(+)} + \tfrac{1}{2} \tag{21}$$

$$E_{+[3/4]}^{(-)}(R) = R^{-2}[3/4]_+^{(-)} + \tfrac{3}{2} \tag{22}$$

where

$$[3/4]_+^{(\pm)} = \frac{a_0^{(\pm)} + a_1^{(\pm)}R^2 + a_2^{(\pm)}R^4 + a_3^{(\pm)}R^6}{1 + b_1^{(\pm)}R^2 + b_2^{(\pm)}R^4 + b_3^{(\pm)}R^6 + b_4^{(\pm)}R^8} \tag{23}$$

with

$$\begin{aligned}
a_0^{(+)} &= 1{\cdot}233\,700\,55 & a_0^{(-)} &= 4{\cdot}934\,802\,201\\
a_1^{(+)} &= -7{\cdot}279\,082\,1\times10^{-1} & a_1^{(-)} &= -1{\cdot}835\,159\,3\\
a_2^{(+)} &= 0{\cdot}131\,651\,36 & a_2^{(-)} &= 1{\cdot}922\,875\,1\times10^{-1}\\
a_3^{(+)} &= -7{\cdot}710\,010\,5\times10^{-3} & a_3^{(-)} &= -3{\cdot}139\,434\,7\times10^{-3}\\
b_1^{(+)} &= -0{\cdot}184\,735\,44 & b_1^{(-)} &= -6{\cdot}791\,747\,0\times10^{-2}\\
b_2^{(+)} &= -2{\cdot}112\,493\,2\times10^{-2} & b_2^{(-)} &= -1{\cdot}031\,957\,7\times10^{-2}\\
b_3^{(+)} &= -5{\cdot}026\,219\,6\times10^{-3} & b_3^{(-)} &= -1{\cdot}827\,751\,2\times10^{-3}\\
b_4^{(+)} &= 4{\cdot}380\,602\,3\times10^{-4} & b_4^{(-)} &= -1{\cdot}469\,584\,1\times10^{-4}.
\end{aligned} \tag{24}$$

With equations (8) and (9) valid for small $R$ and the asymptotic behaviour $E_+^{(+)} \xrightarrow[R\to\infty]{} \frac{1}{2}$ and $E_+^{(-)} \xrightarrow[R\to\infty]{} \frac{3}{2}$, respectively, for the two lowest levels in the case of the harmonic potential, we have constructed the two-point Padé approximants for this case, namely

$$E_{+[4/\!/3]}^{(\pm)}(R) = R^{-2}[4/\!/3]_+^{(\pm)}(z) \qquad z = R^2$$

where

$$[4/\!/3]_+^{(\pm)}(z) = \sum_{i=0}^{4} a_i^{(\pm)} z^i \left(1 + \sum_{i=1}^{3} b_i^{(\pm)} z^i\right)^{-1} \tag{25}$$

with

$$\begin{aligned}
a_0^{(+)} &= 1{\cdot}233\,700\,55 & a_0^{(-)} &= 4{\cdot}934\,802\,201 \\
a_1^{(+)} &= 0{\cdot}322\,774\,61 & a_1^{(-)} &= 2{\cdot}705\,455\,087 \\
a_2^{(+)} &= 9{\cdot}891\,158\,4\times 10^{-2} & a_2^{(-)} &= 2{\cdot}741\,385\,9\times 10^{-1} \\
a_3^{(+)} &= 2{\cdot}002\,187\,3\times 10^{-2} & a_3^{(-)} &= 8{\cdot}815\,545\,7\times 10^{-2} \\
a_4^{(+)} &= 1{\cdot}185\,644\,16\times 10^{-3} & a_4^{(-)} &= 3{\cdot}245\,668\,7\times 10^{-3} \\
b_1^{(+)} &= 0{\cdot}261\,631\,24 & b_1^{(-)} &= 5{\cdot}481\,790\,3\times 10^{-1} \\
b_2^{(+)} &= 2{\cdot}720\,769\,7\times 10^{-2} & b_2^{(-)} &= 2{\cdot}691\,135\,6\times 10^{-2} \\
b_3^{(+)} &= 2{\cdot}371\,283\,2\times 10^{-3} & b_3^{(-)} &= 2{\cdot}163\,779\,2\times 10^{-3}.
\end{aligned} \tag{26}$$

For the inverted potential, with the help of expansions (8) and (9) and the asymptotic expansion (20), we have constructed the two-point [8//5] Padé approximant for $\epsilon(\omega) = R^2E(R)$, where $\omega = R^{4/3}$. Therefore $E_-^{(\pm)}(R)$ can be approximated by

$$E_{-[8/\!/5]}^{(\pm)}(R) = R^{-2}\sum_{i=0}^{8} a_i^{(\pm)}\omega^i\left(1+\sum_{i=1}^{5} b_i^{(\pm)}\omega^i\right)^{-1} = R^{-2}[8/\!/5]_-^{(\pm)} \tag{27}$$

where

$$\begin{aligned}
a_0^{(+)} &= 1{\cdot}233\,700\,55 & a_7^{(+)} &= 3{\cdot}123\,773\times 10^{-3} \\
a_1^{(+)} &= -5{\cdot}586\,822\,3 & a_8^{(+)} &= 6{\cdot}904\,162\,5\times 10^{-5} \\
a_2^{(+)} &= 0{\cdot}125\,021\,77 & b_1^{(+)} &= -4{\cdot}528\,507\,547 \\
a_3^{(+)} &= -9{\cdot}891\,159\,2\times 10^{-2} & b_2^{(+)} &= -0{\cdot}101\,338\,830\,7 \\
a_4^{(+)} &= 0{\cdot}287\,577\,643 & b_3^{(+)} &= -2{\cdot}720\,766\,3\times 10^{-2} \\
a_5^{(+)} &= 6{\cdot}451\,681\,5\times 10^{-3} & b_4^{(+)} &= -6{\cdot}760\,043\,9\times 10^{-3} \\
a_6^{(+)} &= 1{\cdot}185\,642\,1\times 10^{-3} & b_5^{(+)} &= -1{\cdot}380\,832\,5\times 10^{-4}
\end{aligned} \tag{28}$$

for the lowest even state and

$$\begin{aligned}
a_0^{(-)} &= 4{\cdot}934\,802\,201 & a_7^{(-)} &= 4{\cdot}074\,906\,2\times 10^{-4} \\
a_1^{(-)} &= -10{\cdot}318\,409\,51 & a_8^{(-)} &= 3{\cdot}496\,635\,7\times 10^{-6} \\
a_2^{(-)} &= -0{\cdot}896\,665\,61 & b_1^{(-)} &= -2{\cdot}090\,946\,929 \\
a_3^{(-)} &= -0{\cdot}160\,820\,45 & b_2^{(-)} &= -1{\cdot}817\,024\,4\times 10^{-2} \\
a_4^{(-)} &= 0{\cdot}291\,376\,99 & b_3^{(-)} &= -3{\cdot}948\,299\,7\times 10^{-3} \\
a_5^{(-)} &= 2{\cdot}533\,606\times 10^{-3} & b_4^{(-)} &= -8{\cdot}409\,368\,6\times 10^{-4} \\
a_6^{(-)} &= 4{\cdot}199\,977\,1\times 10^{-4} & b_5^{(-)} &= -6{\cdot}993\,271\,5\times 10^{-6}
\end{aligned} \tag{29}$$

for the lowest odd state.

In the next section, we will discuss the results.

**Table 1.** Odd parity levels for the attractive case.

| $R = 0{\cdot}5$ | $R = 1$ | $R = 2$ |
|---|---|---|
| 19·774 534 178 560 | 5·075 582 014 976 | 1·764 816 438 592 |
| 78·996 921 150 976 | 19·899 696 499 3 | 5·584 639 078 1 |
| 177·693 843 822 080 | 44·577 171 227 1 | 11·764 982 120 9 |
| 315·868 612 673 536 | 79·121 980 850 6 | 20·403 520 681 |
| 493·521 634 054 144 | 123·535 750 10 | 31·507 799 34 |
| 710·653 008 064 512 | 177·818 871 88 | 45·078 973 32 |
| 967·262 768 984 064 | 241·971 479 61 | 61·117 342 67 |
| 1 263·350 931 234 816 | 315·993 628 7 | 79·623 013 2 |
| 1 598·917 501 620 224 | 399·885 345 7 | 100·596 030 4 |
| 1 973·962 483 650 560 | 493·646 644 4 | 124·036 416 2 |

| $R = 3$ | $R = 4$ | $R = 5$ | $R = 6$ |
|---|---|---|---|
| 1·506 081 527 088 | 1·500 014 602 7 | 1·500 000 003 5 | 1·499 999 999 |
| 3·664 219 644 | 3·501 691 537 | 3·500 001 22 | 3·499 999 99 |
| 6·473 336 615 | 5·539 421 796 | 5·500 098 71 | 5·500 000 01 |
| 10·303 784 984 | 7·793 679 610 | 7·502 927 99 | 7·500 001 26 |
| 15·229 386 19 | 10·533 684 47 | 9·536 572 97 | 9·500 049 95 |
| 21·254 763 56 | 13·884 832 24 | 11·713 115 18 | 11·501 056 82 |
| 28·378 893 60 | 17·865 148 3 | 14·196 985 9 | 13·512 296 7 |
| 36·600 930 3 | 22·471 738 3 | 17·078 643 2 | 15·579 546 9 |
| 45·920 381 1 | 27·701 207 2 | 20·375 071 6 | 17·804 214 |
| 56·336 962 4 | 33·551 393 2 | 24·082 613 1 | 20·283 577 |

**Table 2.** Even parity levels for the attractive case.

| $R = 0{\cdot}5$ | $R = 1$ | $R = 2$ |
|---|---|---|
| 4·951 129 323 264 | 1·298 459 831 928 | 0·537 461 209 21 |
| 44·452 073 828 864 | 11·258 825 780 608 | 3·399 788 240 |
| 123·410 710 456 832 | 31·005 254 50 | 8·368 874 427 |
| 241·846 458 758 144 | 60·616 003 72 | 15·776 195 797 |
| 399·760 332 976 128 | 100·095 210 78 | 25·647 333 71 |
| 597·152 524 107 776 | 149·443 630 75 | 37·984 998 13 |
| 834·023 089 029 120 | 208·661 485 54 | 52·789 749 77 |
| 1 110·372 049 494 016 | 277·748 859 4 | 70·061 761 6 |
| 1 426·199 415 111 680 | 356·705 790 1 | 89·801 101 8 |
| 1 781·505 191 022 592 | 445·532 296 7 | 112·007 801 3 |

| $R = 3$ | $R = 4$ | $R = 5$ | $R = 6$ |
|---|---|---|---|
| 0·500 391 082 8 | 0·500 000 490 7 | 0·499 999 999 9 | 0·499 999 999 8 |
| 2·541 127 258 | 2·500 201 179 5 | 2·500 000 083 | 2·499 999 998 |
| 4·954 180 470 | 4·509 640 989 | 10·596 191 58 | 4·500 000 00 |
| 8·252 874 649 | 6·621 124 01 | 4·500 012 63 | 6·500 000 15 |
| 12·629 087 15 | 9·091 013 12 | 6·500 602 35 | 8·500 008 6 |
| 18·104 660 9 | 12·130 692 55 | 8·511 471 3 | 10·500 247 7 |
| 24·679 547 4 | 15·796 449 6 | 12·908 515 1 | 12·503 883 2 |
| 32·352 710 8 | 20·090 402 2 | 15·586 086 7 | 14·533 593 4 |
| 41·123 500 2 | 25·008 773 3 | 18·675 121 7 | 16·664 950 5 |
| 50·991 543 0 | 30·548 807 3 | 22·177 796 6 | 19·008 265 4 |

## 5. Exact numerical results

We wish to consider first the variational method, with the trial functions given by equations (6*a*) and (6*b*), which corresponds to the diagonalisation of the Hamiltonian matrix whose elements are given explicitly by equation (7). This is done for several values of $R$ and the corresponding first ten eigenvalues are shown in the tables presented below. The matrix dimension was varied in such a way to guarantee the convergence of the eigenvalues up to the precision shown in the tables.

In table 1 we give the results for the odd parity levels in the attractive case. These correspond to the case studied by Consortini and Frieden (1976). In table 2 we give the results for the even parity states with the boundary condition given by equation (3*a*). In tables 3 and 4 we give the corresponding results for the repulsive case, which correspond to the case studied by Rotbart (1978).

**Table 3.** Odd parity levels for the repulsive case.

| $R=0\cdot25$ | $R=0\cdot5$ | $R=1$ |
|---|---|---|
| 78·948 001 548 800 | 19·703 865 990 976 | 4·792 906 633 984 |
| 315·817 319 989 248 | 78·916 754 105 856 | 19·579 030 856 960 |
| 710·601 276 137 472 | 177·611 917 722 112 | 44·249 466 992 |
| 1 263·299 045 601 280 | 315·786 070 904 832 | 78·791 813 795 |
| 1 973·910 526 857 216 | 493·438 807 326 720 | 123·204 443 176 |
| 2 842·435 694 755 840 | 710·570 026 545 152 | 177·486 945 78 |
| 3 868·874 540 777 472 | 967·179 694 153 728 | 241·639 180 17 |
| 5 053·227 061 379 072 | 1 263·267 795 824 640 | 315·661 086 9 |
| 6 395·493 254 660 096 | 1 598·834 324 635 648 | 399·552 637 8 |
| 7 895·673 119 768 576 | 1 973·879 276 953 600 | 493·313 817 6 |

| $R=1\cdot5$ | $R=2$ | $R=2\cdot5$ | $R=3$ |
|---|---|---|---|
| 1·868 810 529 6 | 0·631 464 302 0 | −0·238 320 840 7 | −1·150 858 051 |
| 8·414 065 072 | 4·304 526 925 | 2·202 110 434 | 0·883 199 16 |
| 19·371 676 57 | 10·454 316 14 | 6·106 763 45 | 3·534 573 36 |
| 34·721 196 19 | 19·082 846 12 | 11·616 438 55 | 7·332 137 15 |
| 54·458 889 17 | 30·182 557 78 | 18·713 974 50 | 12·246 847 95 |
| 78·583 755 59 | 43·751 259 14 | 27·394 380 70 | 18·266 867 17 |
| 107·095 440 24 | 59·788 138 57 | 37·655 777 15 | 25·387 834 67 |
| 139·993 791 86 | 78·292 842 1 | 49·497 330 1 | 33·607 817 9 |
| 177·278 737 3 | 99·265 196 1 | 62·918 625 6 | 42·925 852 5 |
| 218·950 237 8 | 122·705 107 4 | 77·919 439 4 | 53·341 413 |

| $R=3\cdot5$ | $R=4$ | $R=5$ | $R=6$ | $R=7$ |
|---|---|---|---|---|
| −2·297 205 13 | −3·725 604 46 | −7·410 033 4 | −12·165 371 | −17·970 791 |
| −0·122 202 07 | −1·166 966 52 | −4·100 476 2 | −8·218 631 | −13·451 54 |
| 1·806 095 48 | 0·546 767 45 | −1·801 833 3 | −5·302 762 | −10·015 48 |
| 4·535 361 78 | 2·540 498 01 | −0·148 343 9 | −3·011 173 | −7·202 35 |
| 8·116 430 73 | 5·223 984 99 | 1·400 891 0 | −1·215 914 | −4·841 94 |
| 12·522 449 19 | 8·564 768 0 | 3·387 419 7 | 0·198 119 | −2·858 64 |
| 17·743 676 86 | 12·542 000 4 | 5·841 030 9 | 1·674 764 | −1·228 97 |
| 23·775 861 2 | 17·146 881 0 | 8·727 628 1 | 3·512 557 | 0·097 99 |
| 30·616 885 3 | 22·375 079 | 12·031 321 | 5·6950 072 | 1·448 84 |
| 38·265 596 2 | 28·224 242 | 15·743 896 | 8·193 245 | 3·085 93 |

**Table 4.** Even parity levels for the repulsive case.

| $R = 0\cdot25$ | $R = 0\cdot5$ | $R = 1$ |
|---|---|---|
| 19·735 124 564 992 | 4·918 456 569 664 | 1·167 756 672 152 |
| 177·643 166 202 368 | 44·374 369 462 272 | 10·948 019 878 |
| 493·470 056 722 432 | 123·329 403 544 576 | 30·680 027 470 |
| 967·210 943 868 928 | 241·764 159 310 848 | 60·286 805 974 |
| 1 598·865 574 494 208 | 399·677 625 073 664 | 99·764 379 192 |
| 2 388·433 900 699 648 | 597·069 609 463 808 | 149·111 972 13 |
| 3 335·915 908 333 568 | 833·940 055 457 792 | 208·329 351 26 |
| 4 441·311 591 923 712 | 1 110·288 941 318 144 | 277·416 426 74 |
| 5 704·620 948 979 712 | 1 426·116 257 071 104 | 356·373 158 0 |
| 7 125·843 978 280 152 | 1 781·421 998 018 560 | 445·199 524 7 |

| $R = 1\cdot5$ | $R = 2$ | $R = 2\cdot5$ | $R = 3$ |
|---|---|---|---|
| 0·394 174 138 9 | 0·002 263 391 3 | −0·422 041 453 5 | −1·170 473 175 |
| 4·586 822 478 | 2·168 354 461 | 0·898 556 498 | 0·200 106 508 |
| 13·343 368 817 | 7·068 585 566 | 3·951 576 435 | 2·066 066 919 |
| 26·497 796 905 | 14·459 431 801 | 8·662 548 655 | 5·292 329 665 |
| 44·041 608 350 | 24·323 993 505 | 14·967 153 25 | 9·650 876 18 |
| 65·972 955 23 | 36·658 351 74 | 22·856 473 30 | 15·119 052 66 |
| 92·291 257 75 | 51·461 204 82 | 32·327 521 37 | 21·689 885 75 |
| 122·996 288 36 | 68·732 025 80 | 43·379 066 14 | 29·360 523 8 |
| 158·087 943 3 | 88·470 569 8 | 56·010 527 0 | 38·129 618 5 |
| 197·566 169 8 | 110·676 711 0 | 70·221 602 3 | 47·996 465 0 |

| $R = 3\cdot5$ | $R = 4$ | $R = 5$ | $R = 6$ | $R = 7$ |
|---|---|---|---|---|
| −2·297 879 31 | −3·725 613 23 | −7·410 033 4 | −12·165 371 | −17·970 79 |
| −0·319 978 30 | −1·182 241 9 | −4·100 478 3 | −8·218 631 | −13·451 54 |
| 0·815 555 93 | 0·074 039 0 | −1·803 959 6 | −10·015 48 | −10·015 48 |
| 0·306 128 732 | 1·465 416 6 | −0·315 260 5 | −3·011 223 | −7·202 35 |
| 6·221 751 38 | 3·797 839 9 | 0·651 960 6 | −1·226 497 | −4·841 94 |
| 10·217 127 09 | 6·813 958 5 | 2·333 055 8 | −0·083 184 | −2·858 72 |
| 15·031 499 83 | 10·474 530 8 | 4·558 579 9 | 0·922 708 | −1·238 43 |
| 20·658 562 9 | 14·766 319 7 | 7·231 459 | 2·548 068 | −0·134 97 |
| 27·095 355 5 | 19·683 243 3 | 10·327 963 | 4·563 018 | 0·780 79 |
| 34·340 329 8 | 25·222 142 3 | 13·836 848 | 6·905 836 | 2·230 29 |

For all values of $R$ considered, we diagonalise matrices of dimension $35 \times 35$, although for radius up to $R = 1$, lower dimension matrices give the same precision shown in tables 1–4, in particular for the lower energy levels. For instance, 15-dimensional matrices already give the same precision shown in table 4 for the first nine levels in the case $R = 0\cdot25$, and for the first eight levels in the case $R = 0\cdot5$.

In each case we have concentrated our attention on the first ten levels only.

We note that Consortini and Frieden (1976) only considered the odd parity states which correspond to the boundary condition equation (3*b*).

## 6. Results from the perturbative, asymptotic and Padé approximants

In table 5 we give the numerical results for the two lowest energies obtained from the perturbative expansions (8) and (9). By comparison with tables 1–4, we see that the perturbative expansions (8) and (9) give very good results up to $R \sim 1{\cdot}0$.

For the harmonic potential expressions (10) and (11) are reasonable for the lowest levels ($n = 0, 1, 2$) for $R \geqslant 3$, $R \geqslant 4$ and $R \geqslant 5$, respectively, if we compare them with the values given in tables 1 and 2.

In table 6, we give the values of the first four levels obtained from the asymptotic expression (20) obtained for the repulsive case. We see by comparison with tables 3 and 4 that we obtain reasonable results even for the higher levels (the exception being those levels whose energy is close to zero, where large cancellations occur). If we introduce higher-order corrections to equation (20) we will improve the results.

In table 7, we give the numerical results obtained from the one-point Padé approximants [2/5] and [3/4] and the two-point Padé approximants [4//3] for the two lowest levels of the harmonic potential. They are described in § 4 (see equations (21), (22), (23) and (25)).

**Table 5.** Perturbative values for the two lowest levels in the attractive and repulsive cases.

| $R$ | $E_+^{(+)}$ | $E_+^{(-)}$ | $E_-^{(+)}$ | $E_-^{(-)}$ |
|---|---|---|---|---|
| 0·25 | | | 19·735 125 | 78·948 602 |
| 0·5 | 4·951 129 | 19·774 540 | 4·918 457 | 19·703 873 |
| 1·0 | 1·298 469 | 5·076 001 | 1·167 746 | 4·793 327 |
| 2·0 | 0·548 403 | 1·790 769 | 0·007 36 | 0·065 9 |
| 3·0 | 1·244 942 | 1·751 890 | 1·834 3 | −0·856 5 |

**Table 6.** Values of the first four levels in the repulsive case obtained from the asymptotic expansion (10).

| R | $E_1$ | $E_2$ | $E_3$ | $E_4$ |
|---|---|---|---|---|
| 5 | −7·406 62 | −4·067 7 | −1·670 87 | 0·174 38 |
| 6 | −12·163 618 | −8·202 7 | −5·243 70 | −2·855 7 |
| 7 | −17·969 78 | −13·442 6 | −9·983 60 | −7·122 58 |

**Table 7.** Numerical results obtained from the one-point Padé approximants [2/5], [3/4] and the two-point Padé approximants [4//3] for the two lowest levels in the attractive case.

| $R$ | $E^{(+)}_{+[2/5]}$ | $E^{(+)}_{+[3/4]}$ | $E^{(-)}_{+[2/5]}$ | $E^{(-)}_{+[3/4]}$ | $E^{(+)}_{+[4//3]}$ | $E^{(-)}_{+[4//3]}$ |
|---|---|---|---|---|---|---|
| 0·5 | 4·951 129 | 4·951 129 | 19·774 534 | 19·774 534 | 4·951 129 | 19·774 534 |
| 1·0 | 1·298 469 | 1·298 470 | 5·075 595 | 5·075 596 | 1·298 467 | 5·075 591 |
| 2·0 | 0·556 250 | 0·531 791 | 1·786 651 | 1·787 456 | 0·540 352 | 1·768 742 |
| 3·0 | 0·486 835 | 0·503 420 | 1·425 783 | 1·430 954 | 0·526 426 | 1·571 321 |
| 4·0 | 0·495 493 | 0·509 144 | 1·457 521 | 1·462 402 | 0·547 220 | 1·695 013 |
| 5·0 | 0·498 653 | 0·508 278 | 1·482 623 | 1·487 034 | 0·550 096 | 1·768 884 |
| 6·0 | 0·499 570 | 0·505 926 | 1·493 123 | 1·496 669 | 0·544 950 | 1·778 117 |
| 10·0 | | | 1·499 718 | 1·500 839 | 0·522 777 | 1·670 500 |
| 50·0 | | | 1·500 000 | 1·500 003 | 0·501 077 | 1·508 750 |
| 100·0 | | | | 1·500 000 | 0·500 271 | 1·502 203 |

By comparison with the exact results given in tables 1 and 2 we note that for both parity levels up to $R \sim 3$, the results of the three Padé approximants are reasonable. For $R \geqslant 4$ the one-point approximants are better than the two-point Padé approximants.

Finally, in table 8 we give the numerical results for the two lowest levels of the repulsive case with the help of the two-point Padé approximants [8//5] given in equation (27). We see that in this case, by comparison with the exact results given in tables 3 and 4, the two-point Padé approximants [8//5] gives good results for $R \leqslant 1{\cdot}5$. But as we have seen before, the perturbative expansions (8) and (9) also give good results.

For $R \geqslant 1{\cdot}5$, the results are bad and for $R \geqslant 4$ the asymptotic expansion (20) gives much better results.

**Table 8.** Numerical results for the two lowest levels in the repulsive case obtained from the two-point Padé approximants [8//5].

| $R$ | $E^{(+)}_{-[8//5]}$ | $E^{(-)}_{-[8//5]}$ |
|---|---|---|
| 0·25 | 19·735 124 | 78·948 00 |
| 0·5 | 4·918 567 | 19·703 873 |
| 1·0 | 1·167 768 | 4·793 328 |
| 1·5 | 0·394 722 | 1·873 682 |
| 2·0 | 0·001 146 | 0·659 713 |
| 2·5 | −0·338 964 | −0·126 107 |
| 3·0 | −0·801 086 | −0·817 367 |
| 3·5 | −1·484 170 | −1·554 76 |
| 4·0 | −2·476 461 | −2·428 767 |
| 5·0 | −5·578 020 | −4·876 731 |
| 6·0 | −10·175 779 | −8·621 726 |
| 7·0 | −16·087 845 | −13·866 24 |

## Acknowledgments

We thank Hiromi Iwamoto for her help in the numerical computations.

## Appendix

Consider the equation

$$-\tfrac{1}{2}\phi'' + R\zeta\phi = E\phi, \tag{A.1}$$

for two values of $E$, $E_1$ and $E_2$, with the corresponding eigenfunctions $\phi_1$ and $\phi_2$. Let us multiply the equation for $\phi_1$ by $\zeta^k\phi'_2$ and the equation for $\phi_2$ by $\zeta^k\phi'_1$, integrate and sum both of them. In this way, we obtain

$$-\int_0^\infty \zeta^k \frac{\mathrm{d}}{\mathrm{d}\zeta}(\phi'_1\phi'_2)\,\mathrm{d}\zeta = -2R\int_0^\infty \zeta^{k+1}\frac{\mathrm{d}}{\mathrm{d}\zeta}(\phi_1\phi_2)\,\mathrm{d}\zeta + 2\int_0^\infty \zeta^k(E_2\phi'_1\phi_2 + E_1\phi'_2\phi_1)\,\mathrm{d}\zeta. \tag{A.2}$$

For $k \neq 0$, after integration by parts, we obtain

$$k \int_0^\infty \zeta^{k-1} \phi_1' \phi_2' \, d\zeta = 2(k+1)R \int_0^\infty \zeta^k \phi_1 \phi_2 \, d\zeta + 2 \int_0^\infty \zeta^k (E_2 \phi_1' \phi_2 + E_1 \phi_1 \phi_2') \, d\zeta \tag{A.3}$$

It is easy to show that the following identities hold (for $k \neq 0$):

$$\int_0^\infty \zeta^{k-1} \phi_1' \phi_2' \, d\zeta = \zeta^{k-1} \phi_1' \phi_2 \bigg|_0^\infty - (k-1) \int_0^\infty \zeta^{k-2} \phi_1' \phi_2 \, d\zeta + 2E_1 \mathcal{M}_{k-1} - 2R\mathcal{M}_k \tag{A.4}$$

$$\int_0^\infty \zeta^{k-1} \phi_1' \phi_2' \, d\zeta = \zeta^{k-1} \phi_1 \phi_2' \bigg|_0^\infty - (k-1) \int_0^\infty \zeta^{k-2} \phi_1 \phi_2' \, d\zeta + 2E_2 \mathcal{M}_{k-1} - 2R\mathcal{M}_k, \tag{A.5}$$

where we have introduced the notation

$$\mathcal{M}_k = \int_0^\infty \zeta^k \phi_1 \phi_2 \, d\zeta.$$

Expressions (A.4) and (A.5) are obtained by means of integration by parts and use of equation (A.1).

Summing equations (A.4) and (A.5) we obtain

$$\int_0^\infty \zeta^{k-1} \phi_1' \phi_2' \, d\zeta = \tfrac{1}{2} \zeta^{k-2} [\zeta(\phi_1' \phi_2 + \phi_1 \phi_2') - (k-1)\phi_1 \phi_2]_0^\infty + (E_1 + E_2)\mathcal{M}_{k-1} - 2R\mathcal{M}_k + \tfrac{1}{2}(k-1)(k-2)\mathcal{M}_{k-3}. \tag{A.6}$$

Let us make the change $k \to k+2$ in equations (A.4), (A.5) and (A.6). We obtain

$$\int_0^\infty \zeta^{k+1} \phi_1' \phi_2' \, d\zeta = -(k+1) \int_0^\infty \zeta^k \phi_1' \phi_2 \, d\zeta + 2E_1 \mathcal{M}_{k+1} - 2R\mathcal{M}_{k+2} \tag{A.4'}$$

$$\int_0^\infty \zeta^{k+1} \phi_1' \phi_2' \, d\zeta = -(k+1) \int_0^\infty \zeta^k \phi_1 \phi_2' \, d\zeta + 2E_2 \mathcal{M}_{k+1} - 2R\mathcal{M}_{k+2} \tag{A.5'}$$

$$\int_0^\infty \zeta^{k+1} \phi_1' \phi_2' \, d\zeta = (E_1 + E_2)\mathcal{M}_{k+1} - 2R\mathcal{M}_{k+2} + \tfrac{1}{2}k(k-1)\mathcal{M}_{k-1}. \tag{A.6'}$$

Introducing equation (A.6') in equations (A.4') and (A.5'), we obtain

$$\int_0^\infty \zeta^k \phi_1' \phi_2 \, d\zeta = \frac{E_1 - E_2}{k+1} \mathcal{M}_{k+1} - \tfrac{1}{2}k\mathcal{M}_{k-1} \tag{A.7}$$

$$\int_0^\infty \zeta^k \phi_1 \phi_2' \, d\zeta = \frac{E_2 - E_1}{k+1} \mathcal{M}_{k+1} - \tfrac{1}{2}k\mathcal{M}_{k-1}. \tag{A.8}$$

We have used the fact that the brackets in equation (A.6) vanish.

Introducing equations (A.6), (A.7) and (A.8) in equation (A.3), we obtain

$$\frac{2(E_2-E_1)^2}{(k+1)}\mathcal{M}_{k+1}=2R(2k+1)\mathcal{M}_k-2k(E_1+E_2)\mathcal{M}_{k-1}-\tfrac{1}{2}k(k-1)(k-2)\mathcal{M}_{k-3}, \tag{A.9}$$

valid for $k \geqslant 3$.

Similar relations to equation (A.9) have been obtained by Banerjee (1977), who used an operational method in order to derive them. Note, however, that his matrix elements are defined by integration over the whole interval $(-\infty, +\infty)$ while ours are on the half interval $(0, \infty)$.

Although for the derivation above we have used the fact that $k \geqslant 3$, it is easy to see that by using the same steps, equation (A.9) holds for $k = 1, 2$ also (by considering $\mathcal{M}_{-k'}$ finite with $k' = 0, 1, 2, \ldots$). For instance, for $k = 1$, we have

$$\mathcal{M}_{-}=\frac{6R}{(E_2-E_1)^2}\mathcal{M}_1 \tag{A.10}$$

for $E_2 \neq E_1$. Recall that in this case $\mathcal{M}_0 = 0$.

Now equation (A.2) for $k = 0$ gives

$$-\int_0^\infty \frac{\mathrm{d}}{\mathrm{d}\zeta}(\phi_1'\phi_2')\,\mathrm{d}\zeta$$

$$=-2R\int_0^\infty \zeta\frac{\mathrm{d}}{\mathrm{d}\zeta}(\phi_1\phi_2)\,\mathrm{d}\zeta+2\int_0^\infty (E_2\phi_1'\phi_2+E_1\phi_1\phi_2')\,\mathrm{d}\zeta, \tag{A.11}$$

and equations (A.5) and (A.6) for $k = 2$ give

$$\int_0^\infty \zeta\phi_1'\phi_2'\,\mathrm{d}\zeta=-\int_0^\infty \phi_1'\phi_2\,\mathrm{d}\zeta+2E_1\mathcal{M}_1-2R\mathcal{M}_2 \tag{A.12}$$

$$\int_0^\infty \zeta\phi_1'\phi_2'\,\mathrm{d}\zeta=-\int_0^\infty \phi_1\phi_2'\,\mathrm{d}\zeta+2E_2\mathcal{M}_1-2R\mathcal{M}_2. \tag{A.13}$$

Summing these last two equations, we have

$$\int_0^\infty \zeta\phi_1'\phi_2'\,\mathrm{d}\zeta=(E_1+E_2)\mathcal{M}_1-2R\mathcal{M}_2, \tag{A.14}$$

which, when introduced in equations (A.4) and (A.5), produces

$$\begin{aligned}&\int_0^\infty \phi_1'\phi_2\,\mathrm{d}\zeta=(E_1-E_2)\mathcal{M}_1\\&\int_0^\infty \phi_1\phi_2'\,\mathrm{d}\zeta=(E_2-E_1)\mathcal{M}_1.\end{aligned} \tag{A.15}$$

Introducing these expressions in equation (A.11), we obtain

$$\mathcal{M}_1=-\phi_1'(0)\phi_2'(0)/2(E_1-E_2)^2. \tag{A.16}$$

For $E_1 = E_2$ (and $\phi_1 = \phi_2 = \phi$), equation (A.15) give $\int_0^\infty \phi'\phi\,\mathrm{d}\zeta = 0$, and equation (A.11) reduces to

$$\int_0^\infty \phi^2\,\mathrm{d}\zeta=[\phi'(0)]^2/2R. \tag{A.17}$$

Putting

$$\phi_s(\zeta)=N_s\,\mathrm{Ai}(\zeta/a-2a^2\epsilon_s^0), \tag{A.18}$$

with $a^{-3}=2R$, $a_s=-2a^2\epsilon_s^0$, we obtain from equation (A.17)

$$\int_{a_s}^{\infty}\mathrm{Ai}^2(x)\,\mathrm{d}x=[\mathrm{A'i}(a_s)]^2, \tag{A.19}$$

which was found by Castilho-Alcarás and Leal-Ferreira (1975).

Expression (A.10) gives

$$\langle\phi_s|\zeta^2|\phi_{s'}\rangle=\frac{3}{a^3}\frac{\langle\phi_s|\zeta|\phi_{s'}\rangle}{(\epsilon_{s'}^0-\epsilon_s^0)^2} \tag{A.20}$$

and from (A.16), (A.17) and (A.19) we have

$$\begin{aligned}\langle\phi_s|\zeta|\phi_{s'}\rangle&=-\frac{\phi_s'(0)\phi_{s'}'(0)}{2(\epsilon_{s'}^0-\epsilon_s^0)^2}\\&=\frac{N_sN_{s'}\,\mathrm{Ai}(a_s)\,\mathrm{Ai}(a_{s'})}{2a^2(\epsilon_{s'}^0-\epsilon_s^0)^2}\\&=-\tfrac{1}{2}a^{-3}(\epsilon_{s'}^0-\epsilon_s^0)^{-2}.\end{aligned}$$

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