JOURNAL OF COMPUTATIONAL PHYSICS 51, 519–526 (1983)

Note

Accurate Calculation of the Eigenvalues of the $x^2 + \lambda x^2/(1 + gx^2)$ Potential

I. Introduction

In recent years, the solutions of the Schrödinger stationary equation

$$H\Psi = E\Psi, \qquad H = p^2 + V(x), \tag{1}$$

where $p = -id/dx$ and

$$V(x) = x^2 + \lambda x^2/(1 + gx^2), \tag{2}$$

have attracted considerable attention [1–9] due to their applications in a wide variety of problems of physical interest [1, 2].

The ground state and the two first energy levels were first computed by Mitra [1] for a large range of λ and g values (λ, $g = 0$ up to 100) within the variational Rayleigh–Ritz framework. Later on, various authors performed more exact calculations by means of different techniques [3–5]. However, the marked disagreement among different sources is highly significant and it suggests that such results are not as accurate as they claim to be.

The purpose of this work is to present a new alternative procedure to obtain the H eigenvalues. It consists of calculating three quantities which converge towards these eigenvalues. The difference between any two of these quantities is a measure of the error made in the calculation. This peculiar property bestows on the method a complete selfconsistent property and makes it very trusty.

The paper is organized as follows: in Section II we develop briefly the theoretical details related to the method. Then, in Section III it is applied to problem (2) in order to calculate the corresponding eigenvalues for several λ and g values. Finally, the results are compared with values reported previously by different authors and their respective significances are pointed out.

II. Method

Let us consider the eigenvalue problem

$$H\Psi(x) = E\Psi(x), \qquad a \leqslant x \leqslant b, \tag{3}$$

0021-9991/83 $3.00

where $H = p^2 + V(x)$ and

$$\Psi(a) = A\Psi'(a), \tag{4a}$$

$$\Psi(b) = B\Psi'(b). \tag{4b}$$

The constants A and B do not depend on a, b. For the sake of simplicity, we shall assume in what follows that Ψ is normalized

$$\langle \Psi | \Psi \rangle = \int_a^b \Psi^2(x)\, dx = 1. \tag{5}$$

Differentiating (3) with respect to b, multiplying the result by Ψ and integrating between a and b, we obtain (using current quantum mechanical notation)

$$\frac{\partial E}{\partial b} = \left\langle \Psi \left| H \frac{\partial \Psi}{\partial b} \right\rangle - E \left\langle \Psi \right| \frac{\partial \Psi}{\partial b} \right\rangle. \tag{6}$$

The integration by parts of the first term of the right-hand side of (6) leads us to

$$\frac{\partial E}{\partial b} = \left| \Psi' \frac{\partial \Psi}{\partial b} - \Psi \frac{\partial \Psi'}{\partial b} \right|_a^b, \tag{7a}$$

where f' holds for df/dx. Similarly

$$\frac{\partial E}{\partial a} = \left| \Psi' \frac{\partial \Psi}{\partial a} - \Psi \frac{\partial \Psi'}{\partial a} \right|_a^b. \tag{7b}$$

The right-hand side of (7) can be written in a more suitable form by making use of (4). Differentiating (4) with respect to a and b, it follows that

$$\left(\frac{\partial \Psi}{\partial a}\right)(x=a) + \Psi'(x=a) = A\left\{\frac{\partial \Psi'}{\partial a}(x=a) + \Psi''(x=a)\right\}, \tag{8a}$$

$$\left(\frac{\partial \Psi}{\partial b}\right)(x=a) = A\left(\frac{\partial \Psi'}{\partial b}\right)(x=a), \tag{8b}$$

$$\left(\frac{\partial \Psi}{\partial a}\right)(x=b) = B\left(\frac{\partial \Psi'}{\partial a}\right)(x=b), \tag{8c}$$

$$\left(\frac{\partial \Psi}{\partial b}\right)(x=b) + \Psi'(x=b) = B\left\{\frac{\partial \Psi'}{\partial b}(x=b) + \Psi''(x=b)\right\}. \tag{8d}$$

By introducing (8) in (7), we obtain the master equations [10]

$$\frac{\partial E}{\partial b} = \{B^2(V(b) - E) - 1\}\, \Psi'(b)^2, \tag{9a}$$

$$\frac{\partial E}{\partial a} = -\{A^2(V(a) - E) - 1\}\, \Psi'(a)^2. \tag{9b}$$

In this work we are interested only in even potentials so that it is better to consider symmetric intervals ($a = -b < 0$, $A = B$). When these conditions are fulfilled, the two master equations (9) are identical.

When $B = A = 0$, the eigenfunctions of H satisfy Dirichlet (D) boundary conditions

$$H\Psi_n^{\mathrm{D}} = E_n^{\mathrm{D}}\Psi_n^{\mathrm{D}}, \qquad \Psi_n^{\mathrm{D}}(b) = 0, \tag{10}$$

and (9) leads us to the well-known expression [11]

$$\partial E_n^{\mathrm{D}}/\partial b = -\{(\Psi_n^{\mathrm{D}})'\,(x = b)\}^2. \tag{11}$$

Let $\{\Psi_n, E_n\}$ be the discrete set of eigenfunctions and eigenvalues of H when $b \to \infty$; then

$$\lim_{b\to\infty} E_n^{\mathrm{D}}(b) = E_n. \tag{12a}$$

Equations (11) and (12a) state that E_n^{D} decreases monotonically to its limit E_n when $b \to \infty$

$$E_n^{\mathrm{D}} \geqslant E_n. \tag{12b}$$

The quantum mechanical virial theorem [12]

$$-b(\partial E_n^{\mathrm{D}}/\partial b) = 2\langle\Psi_n^{\mathrm{D}} \mid p^2\Psi_n^{\mathrm{D}}\rangle - \langle\Psi_n^{\mathrm{D}} \mid xV'\Psi_n^{\mathrm{D}}\rangle, \tag{13}$$

can be transformed into

$$L_n(b) = E_n^{\mathrm{D}} + (\tfrac{1}{2})(\partial E_n^{\mathrm{D}}/\partial b) = \langle\Psi_n^{\mathrm{D}} \mid (V + xV'/2)\,\Psi_n^{\mathrm{D}}\rangle, \tag{14}$$

by making use of (10). From (11) and (12) we see that

$$L_n < E_n^{\mathrm{D}}, \qquad \lim_{b\to\infty} L_n = E_n. \tag{15}$$

On the other hand, when $B(=A) \to \infty$ the eigenfunctions of H will satisfy von Neumann (N) boundary conditions

$$H\Psi_n^{\mathrm{N}} = E_n^{\mathrm{N}}\Psi_n^{\mathrm{N}}, \qquad (\Psi_n^{\mathrm{N}})'\,(x = \pm b) = 0. \tag{16}$$

In this case the master equations (9) give

$$\partial E_n^{\mathrm{N}}/\partial b = \{V(b) - E_n^{\mathrm{N}}\}\{\Psi_n^{\mathrm{N}}(x = b)\}^2. \tag{17}$$

When $V(x)$ is a monotonous increasing function of $|x|$, it is very easy to deduce that

$$\partial E_0^{\mathrm{N}}/\partial b > 0, \tag{18a}$$

$$\partial E_n^{\mathrm{N}}/\partial b \leqslant 0 \qquad \text{when} \quad b \leqslant b_n \ (n \neq 0), \tag{18b}$$

$$\partial E_n^{\mathrm{N}}/\partial b > 0 \qquad \text{when} \quad b > b_n \ (n \neq 0), \tag{18c}$$

where b_n is the root of $V(b) = E_n^N(b)$. Inequalities (18) can be easily demonstrated from (16) and (17) [13]. From Eqs. (18) and previous assumptions it follows at once that

$$E_n^N(b) \leqslant E_n \qquad \text{if} \quad b \geqslant b_n, \tag{19a}$$

$$\lim_{b\to\infty} E_n^N(b) = E_n. \tag{19b}$$

Equations (12), (15), and (19) are the basis of our method which consists of solving the eigenvalue equations (10) and (16) for such a large b-values that $E_n^D = E_n^N$ holds. Since E_n^D and E_n^N are upper and lower bounds to the eigenvalues E_n, respectively, then the difference $E_n^D - E_n^N$ measures the inaccuracy of the results. Another very useful test of the exactness of the computed eigenvalues is the difference $E_n^D - L_n$.

It seems that L_n is a lower bound to E_n for those particular potential functions considered here, but we cannot prove it except for the ground state. Nevertheless, if L_n is a lower bound or not, is wholly immaterial for our future discussions.

In conclusion, our basic assumption is that the computed eigenvalue is exact up to the last figure that fulfils

$$E_n^D = E_n^N = L_n. \tag{20}$$

This makes the method self-consistent and provides a very good test of accuracy of results.

III. Results and Discussion

After developing the basic ideas of our method, it only remains to solve Eqs. (10) and (16) in order to obtain E_n^D, L_n, and E_n^N. The way of performing it is irrelevant and we shall adopt here the Rayleigh–Ritz (RR) variational method. The most simple basis sets which fulfil the appropriate boundary condition are the sets of eigenfunctions of $H_0 = p^2$

$$H_0\phi_n^D = e_n^D\phi_n^D, \qquad \phi_n^D(\pm b) = 0, \tag{21}$$

$$H_0\phi_n^N = e_n^N\phi_n^N, \qquad (\phi_n^N)'(\pm b) = 0. \tag{22}$$

Because of the form of the potential function (2) we are not able to compute its matrix elements directly but we can perform this calculation through the method reported by Harris *et al.* [14]. Briefly, this method consists of diagonalizing the matrix (x_{ij}) of x (χ_i will denote its eigenvalues)

$$x_{ij} = \langle \phi_i \mid x\phi_j \rangle, \qquad \phi_i \equiv \phi_i^D, \phi_i^N, \tag{23}$$

by means of a similarity transformation T

$$T^{-1}(x_{ij})T = (\chi_i \delta_{ij}), \tag{24}$$

and then computing the matrix of $V(x)$ as

$$(V_{ij}) = T(V(\chi_i)\,\delta_{ij})\,T^{-1}. \tag{25}$$

Of course, V_{ij} is only an approximation to $\langle \phi_i \mid V\phi_j \rangle$, but the results are very good if the matrix is large enough.

When dealing with even potentials (as it is our actual case) it is better to diagonalize x^2 instead of x. Besides, in such a case it is possible to avoid too large matrices by noticing that even and odd functions do not mix.

Although easy to apply, the procedure just described is more time consuming than a straightforward application of the RR variational method [1] and at first sight it might seem that no advantage was obtained. However, all this work makes the method so trustworthy that we can be sure about the accuracy of results. This fact is of great importance if one takes into account the marked disagreement among previous eigenvalue computations [1, 3–5].

The eigenvalues E_n of problem (1)–(2) are exactly known for several particular λ-, g-, and n-values. For example [6, 7],

$$E_0(g) = 1 - 2g \qquad \text{if} \quad \lambda = -2g(2 + g), \tag{26a}$$

$$E_1(g) = 7 + \lambda/g \quad \text{if} \quad \lambda = -2g(2 + 3g). \tag{26b}$$

Table I shows clearly that our numerically computed eigenvalues agree with Eq. (26) up to the eighth decimal place. At the bottom of the table we have added the b-value and the matrix dimension M (equal for all matrices) used to achieve these results.

The M- and b-values employed in this paper are not minimal, but large enough to reach convergence.

TABLE I

Numerical Calculation of Ground State E_0 and First Excited State E_1 of Potential (2) When $\lambda = -2g(2 + g)$ and $\lambda = -2g(2 + 3g)$, Respectively

g	E_0	g	E_1
0.2	0.60000000	0.2	1.80000000
0.4	0.20000000	0.4	0.60000000
0.6	−0.20000000	0.6	−0.60000000
0.8	−0.60000000	0.8	−1.80000000
1.0	−1.0000000	1.0	−3.0000000

Note. $M = 30$, $b = 6$.

In Table II we display the eigenvalues of the Hamiltonian (1)–(2) for a wide range of λ- and g-values. Our results ($E_n^a(M, b)$) satisfy (20) up to the last figure and, in general, agree better with Bessis and Bessis' eigenvalues (E_n^b) [3] than with those reported by Bhagwat (E_n^c) [4].

The two following facts:

(a) our results are in a total agreement with the known exact eigenvalues (Table I),

(b) the quantities E_n^D, L_n, and E_n^N converge to the same limit without violating any theoretical result obtained in Section II, allow us to conclude that our eigenvalues should be exact up to the last figure. Therefore, they should be more accurate than those reported in [3, 4], except for very large (λ, g)-values (say $\lambda = g = 100$), where E_n^D L_n, and E_n^N converge too slowly.

TABLE II

Eigenstates of the Potential (2) for Various λ- and g-Values

n	E_n^a	E_n^b	E_n^c	n	E_n^a	E_n^b	E_n^c
$\lambda = 0.1$, $g = 0.1$				$\lambda = 1$, $g = 0.1$			
	(30,6)				(30,10)		
0	1.04317372	1.04317371	1.043174	0	1.38053180	1.38053180	1.30533
1	3.1200818	3.12008186	3.120089	1	4.0798830	4.07988301	4.079900
2	5.1810948	5.18109479	5.181112	2	6.6679192	6.66791910	6.667938
3	7.2310100	7.23100998	7.231014	3	9.1665674	9.16656747	9.166578
$\lambda = 0.1$, $g = 1$				$\lambda = 1$, $g = 1$			
	(40,7)				(30,6)		
0	1.0241096	1.02418675	1.024112	0	1.23235072	1.23237205	1.232353
1	3.0514902	3.05165067	3.051498	1	3.5073884	3.50742053	3.507397
2	5.0589632	5.05928655	5.058980	2	5.5897790	5.58986086	5.689803
3	7.0648862	7.06549833	7.064899	3	7.6482012	7.64831681	7.648212
$\lambda = 0.1$, $g = 10$				$\lambda = 1$, $g = 10$			
	(40,7)				(40,6)		
0	1.00594390	1.0059428	1.005948	0	1.05929708	1.05929700	1.059298
1	3.0088110	3.0088109	3.008817	1	3.0880908	3.0880908	3.088091
2	5.0082804	5.00828042	5.008291	2	5.0828478	5.0828477	5.082864
3	7.0090376	7.0090376	7.009050	3	7.0903704	7.0903704	7.090384
$\lambda = 0.1$, $g = 100$				$\lambda = 1$, $g = 100$			
	(40,5.5)				(40,5)		
0	1.00084462	1.0008411	1.000855	0	1.008434	1.00844106	1.008465
1	3.0009832	3.0009831	3.000989	1	3.0098322	3.0098317	3.009840
2	5.0009294	5.0009257	5.000936	2	5.0092874	5.0092755	5.009317
3	7.0009845	7.0009845	7.000999	3	7.009846	7.0098449	7.009849

Table continued

TABLE II (*continued*)

Eigenstates of the Potential (2) for Various λ- and g-Values

n	E_n^a	E_n^b	E_n^c	n	E_n^a	E_n^b	E_n^c
$\lambda = 10$, $g = 0.1$				$\lambda = 100$, $g = 0.1$			
	(40,4)				(40,3)		
0	3.2502612	3.25026122	3.250264	0	9.9761800	9.97618009	9.976199
1	9.6190664	9.61906641	9.619087	1	29.781192	29.7811911	29.781266
2	15.729336	15.7293363	15.729379	2	49.292690	49.292905	49.292816
3	21.591006	21.5910055	21.591056	3	68.513062	68.5130522	68.513244
$\lambda = 10$, $g = 1$				$\lambda = 100$, $g = 1$			
	(40,6)				(40,5)		
0	2.7823306	2.782330	2.782331	0	9.3594180	9.35941803	9.359432
1	7.4175058	7.417506	7.417534	1	26.705966	26.705965	26.706007
2	10.701025	10.7010259	10.701033	2	41.441100	41.4410998	41.441139
3	13.388323	13.3883239	13.388354	3	53.839094	53.839093	53.839119
$\lambda = 10$, $g = 10$				$\lambda = 100$, $g = 10$			
	(60,4.5)				(60,5)		
0	1.5800222	1.5800249	1.580028	0	5.7939424	5.793947	5.793965
1	3.879024	3.8790372	3.879039	1	11.5721968	11.572198	11.572215
2	5.833268	5.8327692	5.832771	2	13.6287712	13.62879	13.628777
3	7.902	7.9031549	7.903174	3	15.9984342	15.988706	15.988477
$\lambda = 10$, $g = 100$				$\lambda = 100$, $g = 100$			
	(60,4.5)				(60,4.5)		
0	1.08410	1.0840643	1.084138	0	1.836422	1.8363850	1.836461
1	3.0983176	3.0983170	3.098330	1	3.9831	3.9830992	3.983112
2	5.0927812	5.09276246	5.092807	2	5.928378	5.9283525	5.928395
3	7.0984502	7.0984491	7.098468	3	7.984	7.9844448	7.984464

In Section II we restrict ourselves to dealing with even potentials because we were interested in problem (1)–(2) only. But Eqs. (9) are of a general enough nature to let the method be applied to any one-dimensional quantum mechanical model provided its potential functions do not have singularities in $(-\infty, \infty)$.

The combination of the theoretical conclusions displayed in Section II with the RR variational method is a very helpful procedure to obtain eigenvalues of known accuracy. In those cases where a direct computation of the matrix elements of V is not possible, we can employ the method developed by Harris *et al.* [14] and Endres [15].

REFERENCES

1. A. K. MITRA, *J. Math. Phys.* **19** (1978), 2018.
2. R. S. KAUSHAL, *J. Phys. A Gen. Phys.* **12** (1979), L 253.
3. N. BESSIS AND G. BESSIS, *J. Math. Phys.* **21** (1980), 2780.
4. K. V. BHAGWAT, *J. Phys. A Gen. Phys.* **14** (1981), 377.
5. A. HAUTOT, *J. Comput. Phys.* **39** (1981), 72.
6. V. S. VARMA, *J. Phys. A Gen. Phys.* **14** (1981), L 489.
7. G. P. FLESSAS, *Phys. Lett. A* **83** (1981), 121.
8. G. P. FLESSAS, *J. Phys. A Gen. Phys.* **15** (1982), L 97.
9. R. R. WHITEHEAD, A. WATT, G. P. FLESSAS, AND M. A. NAGARAJAN, *J. Phys. A* **15** (1982), L 1217.
10. F. M. FERNÁNDEZ AND E. A. CASTRO, *Int. J. Quantum Chem.* **19** (1981), 533.
11. I. GONDA AND B. F. GRAY, *J. Chem. Soc. Faraday Trans. 2* **71** (1975), 2016.
12. T. L. COTTRELL AND S. PATERSON, *Philos. Mag.* **42** (1951), 391.
13. F. M. FERNÁNDEZ AND E. A. CASTRO, *Int. J. Quantum Chem.* **21** (1982), 875.
14. D. O. HARRIS, G. G. ENGERHOLM, AND W. D. GWINN, *J. Chem. Phys.* **43** (1965), 1515.
15. P. F. ENDRES, *J. Chem. Phys.* **47** (1967), 798.

RECEIVED: August 31, 1982; REVISED : December 3, 1982

FRANCISCO M. FERNÁNDEZ, ALEJANDRO M. MESÓN,
AND EDUARDO A. CASTRO

INIFTA, Sección Química Teórica,
Sucursal 4, Casilla de Correo 16,
La Plata 1900, Argentina