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Application of the eigenvalue moment method to important one-dimensional quantum systems

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Abstract. We study the effectiveness of the eigenvalue moment method as applied to various one-dimensional quantum problems which have appeared in the literature. Of particular interest are the radial potential problems (including angular momentum effects) $-Ze^2/(r + \beta)$ and $r^2 + \lambda r^2/(1 + gr^2)$ studied by De Meyer and Vanden Berghe (and more recently by Fernandez), and Witwit, respectively. We also examine the potentials $\frac{1}{2}x^2 \pm gx^4/(1 + \alpha gx^2)$, exhaustively studied by Auberson and Boissiere. Finally, we examine the one-dimensional regulated Bohr atom with potential $-Z/(|x| + \alpha)$, well studied by Loudon, and Haines and Roberts.

1. Introduction

The eigenvalue moment method (EMM) is a general theory for generating converging lower and upper bounds to the low-lying discrete spectrum of arbitrary, bosonic, Schrödinger equation Hamiltonians (Handy and Bessis 1985, Handy *et al* 1988a, b, 1991a, b). It has enjoyed some notable successes in significantly confirming high-precision eigenenergy estimates, as well as in refuting some published results.

One instance of the former is the application to the superstrong magnetic field regime for the quadratic Zeeman effect (Handy *et al* 1988a, b), confirming the order-dependent conformal transformation analysis of Le Guillou and Zinn-Justin (1983).

An example of an erroneous result is the Hellman–Feynman hypervirial estimate of Lai and Lin (1982) for the $x^2 + \lambda x^2/(1 + gx^2)$ potential, particularly for parameter values $\lambda = 0.1$ and $g = 2$. For this case, their analysis yielded 1.017 281 60 for the ground-state energy. The EMM bounds gave $1.017 176 < E_g < 1.017 185$ clearly invalidating the Lai and Lin estimate, at the fourth decimal place. The EMM bounds were subsequently confirmed through a more specialized analysis by Hodgson (1988).

A second example, although not as severe, is the EMM analysis of the quartic anharmonic oscillator, $-Z^2x^2 + x^4$, as studied by de Saavedra and Buendia (1990). For the $Z^2 = 5$ case, the numerical stability properties of the EMM approach, as discussed by Handy (1992), yielded the ground-state energy bounds $-3.410 142 761 239 829 50 < E_g < -3.410 142 761 239 829 35$, subsequently reconfirmed (typographical error) by de Saavedra and Buendia (1992).

The EMM approach has been applied to many one- and two-dimensional problems. However, until now, it has not been applied to cases involving non-zero angular momentum.

The recent analysis by De Meyer and Vanden Berghe (1990), and Fernandez (1991) of the $-Ze^2/(r + \beta)$ radial potential, as well as the work of Witwit (1991) with respect to the $r^2 + \lambda r^2/(1 + gr^2)$ problem, compel us to investigate the relevance of an EMM analysis in such cases. We also study another problem investigated by Witwit (1991), that corresponds to the potential $\frac{1}{2}x^2 \pm gx^4/(1 + \alpha gx^2)$; however, our interest is in contrasting the EMM results with the Borel resummation results of Auberson and Boissiere (1983). Finally, we also discuss the EMM analysis for the one-dimensional regulated Bohr atom $-Z/(|x| + \alpha)$, for $\alpha \rightarrow 0$. This problem is of interest because it may suggest alternative EMM representations by which to improve the binding energy bounds for the superstrong quadratic Zeeman effect (Handy *et al* 1988a, b).

It is well recognized that bounding theories (those generating lower and upper eigenenergy bounds) can be very demanding theoretically and computationally. Accordingly, we do not expect EMM theory to be computationally competitive with most other eigenenergy methods. However, it can be argued that EMM is a reliable and simple theory that can be used to test the reliability or accuracy of other faster, but potentially less precise, methods. The cases examined in this work support this point of view.

2. The $-Ze^2/(r + \beta)$ potential

Consider the Schrödinger equation for a *cut-off* Coulombic potential, as studied by De Meyer and Vanden Berghe (1990)

$$-\frac{1}{2} \frac{d^2\Psi}{dr^2} + \left[\frac{1}{2} \frac{l(l+1)}{r^2} - \frac{Ze^2}{r+\beta} \right] \Psi(r) = E\Psi(r) \quad (2.1)$$

where l is the angular momentum, and $Ze^2 \equiv 1$ is the product of the electrical charges. In addition, the radial wavefunction satisfies

$$\Psi(0) = 0. \quad (2.2)$$

For clarity of presentation, we will limit all discussions in this work to the ground-state solution within each symmetry class (corresponding to different l values). The analysis of excited states can be pursued through the c -shift EMM methods of Handy and Lee (1991). The present problem will serve as an introduction to EMM theory, which is discussed in greater detail in the cited references.

The basic EMM analysis proceeds by first transforming equation (2.1) into a moment equation representation. This is accomplished by multiplying both sides of equation (2.1) by $r^2(r + \beta)$ and integrating by parts with respects to $\int_0^{+\infty} r^p dr$. Although the resulting moment equation would also be valid for the $l = 0$ and $\beta = 0$ cases, our experience suggests that no good eigenenergy bounds would result for reasons to be presented elsewhere. Accordingly, for these special cases, one would only multiply both sides of the corresponding Schrödinger equation by either $(r + \beta)$ or r^2 . That is, the following formalism should only be used for $l \geq 1$ and $\beta \neq 0$.

There are two important considerations before generating an appropriate moment equation. The first is

$$\int_0^{+\infty} r^p \Psi(r) dr < \infty \quad \text{if } p \geq -1 \quad (2.3)$$

as follows from equation (2.2) and the exponentially decreasing nature of bound-state solutions. The second is that the *integration by parts* of equation (2.1) will yield boundary terms of the type

$$\int_0^{+\infty} r^p \Psi''(r) dr = -\delta_{p,0} \Psi'(0) + p(p-1)u(p-2) \quad p \geq 0 \quad (2.4)$$

where $u(p)$ is the p th-order Stieltjes moment $u(p) = \int_0^{+\infty} r^p \Psi(r) dr$. There will be no boundary terms if $p \geq -1$, for the case $\beta \neq 0$ ($p \geq -2$ if $\beta = 0$). It then becomes appropriate to work with the shifted moments $w(p) \equiv u(p-1)$, for $p \geq 0$ ($w(p)$ will retain this definition throughout this work).

The resulting moment equation is

$$-2Ew(p+3) = [2\beta E + 2]w(p+2) + [(p+2)(p+1) - \gamma]w(p+1) + \beta[p(p+1) - \gamma]w(p) \quad (2.5)$$

where $\gamma = l(l+1)$ and $p \geq 0$.

This moment equation corresponds to a third-order *missing moment problem* (Handy and Bessis 1985) in which $w(0)$, $w(1)$ and $w(2)$ must be specified before the remaining moments can be generated. Clearly, its homogeneous structure allows us to impose the normalization condition $w(0) + w(1) + w(2) = 1$, resulting in a second-order system, with respect to the unconstrained missing moments. All references in this work to the *unconstrained missing moment order* will refer to the effective order after imposing the appropriate normalization condition.

Eliminating $w(0)$ we can express the linear dependence of all the moments on the unconstrained missing moments ($w(1)$ and $w(2)$) through the relations

$$w(p) = \sum_{l=0}^2 \hat{M}_E(p, l) \hat{w}(l) \quad (2.6)$$

where $\hat{w}(0) \equiv 1$ and $\hat{w}(i \neq 0) \equiv w(i)$. The energy, E , dependent $\hat{M}_E(p, l)$ coefficients can be easily generated numerically (Handy *et al* 1988a, b).

The derived moment equation is valid for all physical solutions. In order to quantize the ground-state configurations, we must make use of the positivity properties of such configurations so as to define corresponding positivity constraints on the moments. It is a well known theorem that bosonic ground-state wavefunctions are of uniform signature and can be taken to be positive (that is non-negative, in the r -representation: $\Psi_{gr}(r) \geq 0$). The mathematical theorems from the classic *moment problem* (Shohat and Tamarkin 1963) prescribe powerful non-linear inequality moment constraints sufficient to quantize the ground-state energies (Handy and Bessis 1985). However, practically, it is too difficult to solve these non-linear relations directly. Instead, through the use of a linear programming (LP; Chvatal 1983) based *cutting* algorithm (Handy *et al* 1988a, b) it is possible to solve these relations; thereby leading to the quantization of the ground states.

The result of such an LP analysis, for the case $\beta = 1$ and $l = 1$ is $-0.0831 < E_g < -0.0824$, on the basis of working with a maximum moment order, P_{max} , of 28. For the case $\beta = 0.1$ and $l = 1$ we obtain $-0.1178 < E_g < -0.1148$, for $P_{max} = 34$. Similarly, for the case $\beta = 10^{-4}$ and $l = 1$ we obtain $-0.125 < E_g < -0.120$, for $P_{max} = 34$. For these three cases De Meyer and Vanden Berghe (1990) obtain -0.0828624204409 , -0.117535 and -0.124992 respectively. Clearly then, the EMM results are poor.

Better bounds can be obtained through the special transformation

$$\Phi(r) = \Psi(r) \exp(-\sqrt{-2E}r) \quad (2.7)$$

for $E < 0$. One must be careful in choosing such transformations (Handy and Lee 1991). The basic guidelines are: in transforming from $\Psi(r)$ to $\Phi(r) = \Psi(r)R(r)$ one wants a positive function, $R(r) > 0$, whose asymptotic properties (as determined from a zeroth-order JWKB analysis) result in unphysical $\Phi(r)$ configurations (unbounded functions with infinite Stieltjes moments) for unphysical $\Psi(r)$ s; while for the physical $\Psi(r)$ one also wants the corresponding $\Phi(r)$ to be physical (with finite Stieltjes moments).

The corresponding differential equation for $\Phi(r)$ is

$$\frac{d^2\Phi}{dr^2} + 2\sqrt{-2E}\frac{d\Phi}{dr} + \left[-\frac{l(l+1)}{r^2} + \frac{2}{r+\beta} \right] \Phi(r) = 0. \quad (2.8)$$

Repeating the moment equation analysis (absence of boundary terms, etc) the Φ -moment equation becomes ($u(p) = \int_0^{+\infty} r^p \Phi(r) dr \equiv w(p+1)$):

$$[2 - 2\sqrt{-2E}(p+2)]w(p+2) = [\gamma - (p+1)(p+2 - 2\sqrt{-2E}\beta)]w(p+1) - \beta[p(p+1) - \gamma]w(p) \quad (2.9)$$

where $p \geq 0$, and $\beta \neq 0$. Note that this equation involves one less missing moment than that for equation (2.5).

Implementing the linear programming cutting analysis, we obtain the improved results in table 1.

Table 1. E_g bounds for $-1/(r+\beta)$.

β	l	E_g bounds
10^{-4}	1	$-0.1250 < E_g < -0.1244$ [34] ^a (-0.124992) ^b
0.1	1	$-0.11759 < E_g < -0.11727$ [32] (-0.117535)
1	1	$-0.082864 < E_g < -0.08285$ [30] ($-.0828624204409$)
15	1	$-.0228255784915201 < E_g < -0.0228255784915032$ [30] (-0.0228255784915)

^a P_{\max} .

^b De Meyer and Vanden Berghe (1990) results.

The results are clearly superior to the previous bounds. All these results were obtained on an IBM RISC 6000 model 560 in double precision.

For completeness, we discuss the case $\beta = 0$. Again, we work with the same equation (2.8); however, in obtaining a moment equation, it is only necessary to multiply both sides of equation (2.1) by r^{p+2} . Once again, we may take $p \geq -1$, and work with the $w(q = p+1)$ moments, for $q \geq 0$. The moment equation becomes

$$2[(q+1)\sqrt{-2E} - 1]w(q+1) = [q(q+1) - l(l+1)]w(q) \quad \text{for } q \geq 0. \quad (2.10)$$

The above equation corresponds to a zero missing moment problem, since one can set $w(0) \equiv 1$. It then follows that all the other moments are functions of $-E$. The physical

solution must satisfy this moment relation; however, the ground-state moments must be (strictly) positive. We see that when $q = l$, it follows that $w(l + 1) = 0$, unless the coefficient $[(l + 1)\sqrt{-2E} - 1] = 0$. Only for the latter case will there be consistency with the requirement that the physical moments must be finite and positive. Accordingly, we obtain the correct ground state quantization condition,

$$E = -\frac{1}{2}(l + 1)^{-2}. \quad (2.11)$$

3. The $mr^2 + \lambda r^2/(1 + gr^2)$ potential

Consider the problem

$$-\frac{d^2\Psi}{dr^2} + \left[\frac{l(l + 1)}{r^2} + mr^2 + \frac{\lambda r^2}{1 + gr^2} \right] \Psi(r) = E\Psi(r) \quad (3.1)$$

studied by Roy *et al* (1988) and Witwit (1991). We may transform it through $\Phi(r) = \exp(-\alpha r^2)\Psi(r)$ ($-\sqrt{m}/2 < \alpha \leq \sqrt{m}/2$ (Handy and Lee 1991)), into

$$-\left[\frac{d^2\Phi}{dr^2} + 4\alpha r \frac{d\Phi}{dr} + 2\alpha\Phi(r) \right] + \left[\frac{l(l + 1)}{r^2} + \frac{\lambda r^2}{1 + gr^2} \right] \Phi(r) = E\Phi(r) \quad (3.2)$$

where we have chosen $\alpha = \sqrt{m}/2$. The associated Stieltjes moment equation is

$$\begin{aligned} u(p + 4)[Eg - 4\alpha g(p + 5) + 2\alpha g - \lambda] \\ = u(p + 2)[-E - 2\alpha + 4\alpha(p + 3) - g(p + 4)(p + 3) + gl(l + 1)] \\ + u(p)[l(l + 1) - (p + 2)(p + 1)]. \end{aligned} \quad (3.3)$$

We require that $p \geq -1$ in order to avoid boundary terms, as discussed in the previous section.

Clearly, the even- and odd-order Stieltjes moments separate. Because the lowest order $u(p)$ moment possible is that for $p = -1$, we will first examine the consequences of working with the odd-order moments. We can set $u(2\eta - 1) \equiv w(\eta)$, for $\eta \geq 0$. The $w(\eta)$ are also the moments of a Stieltjes measure: $u(2\eta - 1) \equiv \int_0^{+\infty} r^{2\eta-1}\Phi(r) dr = \int_0^{+\infty} \rho^{\eta-1}\frac{1}{2}\Phi(\sqrt{\rho}) d\rho$, through a simple change of variables ($r \equiv \sqrt{\rho}$). The $w(\eta)$ moment equation becomes

$$\begin{aligned} w(\eta + 2)[Eg - 2g\sqrt{m}(2\eta + 4) + g\sqrt{m} - \lambda] = w(\eta + 1)[-E - \sqrt{m} + 2\sqrt{m}(2\eta + 2) \\ - g(2\eta + 3)(2\eta + 2) + gl(l + 1)] + w(\eta)[l(l + 1) - 2\eta(2\eta + 1)] \quad \text{for } \eta \geq 0. \end{aligned} \quad (3.4)$$

3.1. Generating bounds for the $l = \text{even}$ states

The preceding analysis gave very good bounds for the $l = \text{even}$ states. These are given in tables 2 and 3. We compare the EMM bounds with the results of Roy *et al* (1988) for the $m = 1$ case. We do not quote Witwit's (1991) results since his estimates surpass the bounds generated except for one typographical error (we believe) corresponding to $\lambda = 1000$, $g = 0.1$, and $l = 10$. Also, in order to avoid too large numbers (particularly in the case of Witwit's parameter values) we rescaled the moment equation according to $E_g s^2 \equiv E'_g$, $ms^4 \equiv m'$, $s^2 \equiv g'$ and $\lambda s^4 \equiv 1$.

Although satisfactory bounds were also generated for the $l = \text{odd}$ states, these generally produced bounds no tighter than $O(10^{-3})$; thereby motivating the analysis of the even-*Stieltjes* moment case for equation (3.3), as carried out below.

The structure of the moment equation in equation (3.4) offers an explanation as to why better bounds for the even angular momentum states are to be expected. In particular, note that the coefficient $[l(l+1) - 2\eta(2\eta+1)]$ will be zero for $2\eta = l(\text{even})$. One then has

$$\begin{aligned} w(\tfrac{1}{2}l+2)[Eg - 2g\sqrt{m}(l+4) + g\sqrt{m} - \lambda] \\ = w(\tfrac{1}{2}l+1)[-E - \sqrt{m} + 2\sqrt{m}(l+2) - g(l+3)(l+2) + gl(l+1)]. \end{aligned}$$

Since the physical solution must have all its w moments finite and positive, it is clear that both coefficients must be of the same signature. A little algebra yields the relations

$$(\lambda/g) + \sqrt{m}(2l+7) \leq E_g \leq -4gl - 6g + \sqrt{m}(2l+3) \quad (3.5)$$

or

$$(\lambda/g) + \sqrt{m}(2l+7) \geq E_g \geq -4gl - 6g + \sqrt{m}(2l+3)$$

for $l = \text{even}$. If we equate the bounds, we obtain a condition on the parameters leading to an exact solution for the energy: For $\lambda = -[4g^2(l+1) + 2g^2 + 4g\sqrt{m}]$ then

$$E_g = \frac{\lambda}{g} + (2l+7)\sqrt{m}.$$

Although we have set $l = \text{even}$, the above relation holds for all l . One can see this by repeating the above analysis with respect to the moment equation in equation (3.6), as described below. The results agree with those of Roy *et al* (1988, equation (49)).

3.2. Generating bounds for the $l = \text{odd}$ states

The preceding results suggest that the $u(p = \text{even})$ moments may be very relevant for obtaining more precise eigenenergy bounds for the $l = \text{odd}$ states. Indeed, this is the case. More remarkably, the $l = 1$ states 'decouple' from the $l_{\text{odd}} \geq 3$ states. To see this, note that by simply setting $u(2\eta) \equiv v(\eta)$ (in equation (3.3)), for $\eta \geq 0$ we obtain the moment equation

$$\begin{aligned} v(\eta+2)[Eg - 2g\sqrt{m}(2\eta+5) + g\sqrt{m} - \lambda] \\ = v(\eta+1)[-E - \sqrt{m} + 2\sqrt{m}(2\eta+3) - g(2\eta+4)(2\eta+3) + gl(l+1)] \\ + v(\eta)[l(l+1) - (2\eta+1)(2\eta+2)] \quad \text{for } \eta \geq 0. \end{aligned} \quad (3.6)$$

So long as $l_{\text{odd}} \geq 3$, the $[l(l+1) - (2\eta+1)(2\eta+2)]$ coefficient will not be zero for $\eta = 0$. In such cases, the number of (unconstrained) missing moments (after normalization) will be one. However, if $l = 1$, then this coefficient is zero for $\eta = 0$. That is, for $\eta = 0$ and $l = 1$, we will have $v(2)$ solely depending on $v(1)$, with the ensuing recursion relation not involving $v(0)$ at all. Thus, we can really work with the moments $v(\rho+1) \equiv t(\rho)$, for $\rho \geq 0$. The ensuing zero missing moment equation then becomes

$$t(\rho+1)[Eg - 2g\sqrt{m}(2\rho+5) + g\sqrt{m} - \lambda] = t(\rho)[-E - \sqrt{m} + 2\sqrt{m}(2\rho+3) - g(2\rho+4)(2\rho+3) + 2g] + t(\rho-1)[2 - (2\rho+1)(2\rho+2)] \quad \text{for } \rho \geq 0. \quad (3.7)$$

The improved bounds, on the basis of using equations (3.6) and (3.7), are given in tables 2 and 3.

4. The $\frac{1}{2}x^2 \pm gx^4 / (1 + \alpha gx^2)$ potential

4.1. One missing moment formulation

Consider the potential problem

$$-\frac{1}{2} \frac{d^2\Psi}{dx^2} + \left[\frac{1}{2}x^2 \pm \frac{gx^4}{1 + \alpha gx^2} \right] \Psi(x) = E\Psi(x) \quad (4.1)$$

studied by Auberson and Boissiere (1983) with respects to large- g Borel resummation methods. Upon multiplying both sides by the denominator expression $1 + \alpha gx^2$ and integrating over the real axis with respects to x^p , there results the following equation for the Hamburger moments ($\mu(p) \equiv \int_{-\infty}^{+\infty} x^p \Psi(x)$):

$$g[\frac{1}{2}\alpha \pm 1]\mu(p+4) = [E\alpha g - \frac{1}{2}]\mu(p+2) + [\alpha g(\frac{1}{2}p+1)(p+1) + E]\mu(p) + \frac{1}{2}p(p-1)\mu(p-2). \quad (4.2)$$

The symmetric nature of the ground-state wavefunction allows us to simplify the above and work directly with Stieltjes moments, $u(p) \equiv \int_0^{+\infty} r^{p-1/2}\Psi(\sqrt{r})dr$. That is, the even-order Hamburger moments are equivalent to Stieltjes moments: $\mu(2p) \equiv u(p)$. The corresponding Stieltjes moment equation becomes

$$g[\frac{1}{2}\alpha \pm 1]u(p+2) = [E\alpha g - \frac{1}{2}]u(p+1) + [\alpha g(p+1)(2p+1) + E]u(p) + p(2p-1)u(p-1). \quad (4.3)$$

It will be noted that this is a one missing moment problem, so long as $\alpha \neq 2$, for the 'negative' potential case. The latter corresponds to a zero missing moment problem and is examined in the context of equation (4.4). Usually, if one is able to reduce the number of missing moments in a problem, better converging bounds will result. This is possible in the present situation.

Table 2. E_g bounds for $r^2 + \lambda r^2/(1 + gr^2)$.

λ	g	l	E_g bounds: $l = 1$ (equation (3.6)); $l = 3$ (equation (3.7))
0.1	0.1	1	5.186 373 002 9314 < E_g < 5.186 373 002 9316 [30] ^a (5.186 338) ^b
		2	7.243 961 840 4138 < E_g < 7.243 961 840 4260 [30] (7.243 927)
		3	9.294 359 110 863 37 < E_g < 9.294 359 110 881 59 [30]
0.1	0.5	1	5.100 842 < E_g < 5.100 865 [30] (5.100 976)
		2	7.118 90 < E_g < 7.119 01 [30] (7.119 005)
		3	9.131 799 < E_g < 9.131 838 [30]
0.1	1	1	5.064 28 < E_g < 5.066 09 [30] (5.065 610)
		2	7.0730 < E_g < 7.074 4 [30] (7.073 713)
		3	9.0787 < E_g < 9.0792
0.5	0.1	1	5.893 595 152 339 19 < E_g < 5.893 595 152 339 45 [34] (5.893 494)
		2	8.177 871 693 435 < E_g < 8.177 871 693 485 [30] (8.177 754)
		3	10.429 204 118 1366 < E_g < 10.429 204 118 1548 [34]
1	0.1	1	6.704 238 892 4777 < E_g < 6.704 238 892 4788 [34] (6.704 090)
		2	9.261 914 7807 < E_g < 9.261 914 7809 [30] (9.261 812)
		3	11.760 620 962 6312 < E_g < 11.760 620 962 6917 [32]
1	1	1	5.6503 < E_g < 5.6521 [33] (5.652 112)
		2	7.734 < E_g < 7.736 [30] (7.734 778)
		3	9.7875 < E_g < 9.7881 [31]
10	0.1	1	15.813 709 4349 < E_g < 15.813 709 4352 [34] (15.813 628)
		2	21.836 092 467 < E_g < 21.836 092 544 [30] (21.836 043) ^b
		3	27.688 302 83 < E_g < 27.688 302 88 [30]
100	0.1	1	49.389 794 27 < E_g < 49.389 794 34 [30] (49.389 615)
		2	68.802 0606 < E_g < 68.802 0615 [30] (68.801 562)
		3	88.018 0658 < E_g < 88.018 0660
100	10	1	1.7 < E_g < 14.609 [30] (14.363 739)
		2	16.5997 < E_g < 16.65402 [30] (16.611 028)
		3	18.7186 < E_g < 18.7307 [30]
100	100	1	— < E_g < 6.389 [30] (5.993 565)
		2	7.9947 < E_g < 8.037 800 [30] (7.996 048)
		3	9.9969 < E_g < 10.0113 [29]

^a P_{\max} .^b Roy et al (1988).

Table 3. E_g bounds for $r^2 + \lambda r^2/(1 + gr^2)$.

λ	g	l	E_g bounds
200	0.1	5	$179.483\ 107 < E_g < 179.483\ 116$ [33] ^a
200	0.1	10	$311.860\ 1371 < E_g < 311.861\ 6266$ [30]
500	0.1	5	$286.130\ 73 < E_g < 286.130\ 82$ [30]
500	0.1	20	$914.365\ 40 < E_g < 914.368\ 51$ [27]
1000	0.1	10	$713.360\ 81 < E_g < 713.363\ 21$ [31]
1000	0.1	20	$1312.250\ 06 < E_g < 1312.253\ 33$ [28]
1000	0.2	5	$401.6078 < E_g < 401.6081$ [31]
1000	0.2	10	$699.104\ 24 < E_g < 699.109\ 092$ [31]
10 000	0.4	5	$1280.6254 < E_g < 1280.6256$ [32]
10 000	0.4	10	$2242.789\ 1995 < E_g < 2242.789\ 3867$ [32]
10 000	0.5	5	$1275.7838 < E_g < 1275.7842$ [32]
10 000	0.5	10	$2228.513\ 255 < E_g < 2228.530\ 746$ [31]

^a P_{\max} .

4.2. Zero missing moment formulation

The zeroth-order asymptotic behaviour (so long as $\alpha \neq 2$, for the ‘negative’ potential case) is given by $\Psi(x) \rightarrow \exp(\pm \frac{1}{2}\gamma x^2)$, where $\gamma \equiv (1 \pm 2/\alpha)^{1/2}$. A zero missing moment problem results upon performing the transformation $\Phi(x) = \Psi(x) \exp(-\frac{1}{2}\gamma x^2)$:

$$v(p + 1)[2E\alpha g - 1 + \gamma^2 - 2\alpha g\gamma(2p + 3) + \alpha g\gamma] = v(p)[-2E - \gamma + 2\gamma(2p + 1) - g\alpha(2p + 2)(2p + 1)] - v(p - 1)2p(2p - 1) \tag{4.4}$$

where $v(p) \equiv \int_0^{+\infty} r^{p-\frac{1}{2}} \Phi(\sqrt{r}) dr$. Note that for the ‘negative’ potential, when $\alpha = 2$ then $\gamma = 0$. Thus, equation (4.4) becomes exactly equation (4.3) in this special case.

In table 4 we tabulate the numerical results obtained from the moment relations in equations (4.3) and (4.4). An examination of the results clearly shows that, in general, the zero missing moment results (referenced by a superscripted [0]) are superior to those of the one missing moment formulation (as referenced by the [1] notation). Indeed, the $\alpha = 0.1$ results are vastly superior to those quoted by Auberson and Boissiere. This behaviour becomes dramatically reversed at $\alpha = 1$, with some improvement for $\alpha = 2$.

The superiority of the zero missing moment formulation over the one missing moment case suggested that we only implement the former with respect to the ‘negative’ potential. These results are quoted in table 5. Clearly, they are not consistently satisfactory in comparison with the Auberson and Boissiere results. To remedy the situation, we pursued a Hausdorff moment formulation, as discussed below.

4.3. Hausdorff moment formulation

The complex singularities for the rational fraction potential in equation (4.1), $x = \pm i1/\sqrt{\alpha g}$, will affect the tightness of the bounds, particularly as the poles get closer to the real axis or $\alpha g \rightarrow \infty$. It has been shown by Handy *et al* (1988c) that mapping the singularities to infinity improves the tightness of the bounds. This can be done by transforming the preceding Stieltjes moment problem into a Hausdorff moment problem through the transformation $z = x\sqrt{\alpha g}/\sqrt{1 + \alpha g x^2}$. The corresponding differential equation is

$$\left[(1 - z^2)^4 \frac{d^2\Psi}{dz^2} - 3z(1 - z^2)^3 \frac{d\Psi}{dz} \right] - \frac{z^2}{(\alpha g)^2} \left[1 \pm \frac{2}{\alpha} z^2 \right] \Psi(z) = \frac{-2E}{\alpha g} [1 - z^2] \Psi(z) \tag{4.5}$$

Table 4. E_g bounds for potential $\frac{1}{2}x^2 + gx^4/(1 + \alpha gx^2)$.

α	g	E_g bounds
0.1	0.1	$0.558\,233\,730\,598 < E_g < 0.558\,233\,730\,600^{[1]}$ [28] ^a (0.558 233 73) ^{AB}
0.1	1	$0.784\,971\,078\,122 < E_g < 0.784\,971\,078\,127^{[0]}$ [12] $0.784\,971\,0779 < E_g < 0.784\,971\,0785^{[1]}$ [28] (0.784 97)
0.1	2	$0.911\,409\,037\,600\,13 < E_g < 0.911\,409\,037\,600\,18^{[0]}$ [15] $0.911\,409\,0333 < E_g < 0.911\,409\,0394^{[1]}$ [28] (0.911)
0.1	5	$1.122\,987\,571\,5016 < E_g < 1.122\,987\,571\,5018^{[0]}$ [24] $1.122\,987\,56 < E_g < 1.122\,987\,59^{[1]}$ [28] (1.12)
0.1	10	$1.310\,303.4929 < E_g < 1.310\,303\,4931^{[0]}$ [28] $1.310\,3026 < E_g < 1.310\,304\,74^{[1]}$ [28] (1.30)
0.1	15	$1.426\,1759 < E_g < 1.426\,1763^{[0]}$ [28] $1.425\,863 < E_g < 1.42\,6599^{[1]}$ [28] (1.42)
0.1	20	$1.509\,1769 < E_g < 1.509\,1848^{[0]}$ [28] $1.5067 < E_g < 1.5123^{[1]}$ [28] (1.50)
1	2	$0.7293 < E_g < 0.7343^{[0]}$ [28] ^a $0.63 < E_g < 0.85^{[1]}$ [28] (0.731) ^{AB}
1	5	$0.5714 < E_g < 0.9767^{[0]}$ [28] (0.784)
2	0.1	$0.545\,401\,812\,407\,99 < E_g < 0.545\,401\,812\,410\,27^{[0]}$ [27] (0.545 4017)
2	0.2	$0.568\,9417 < E_g < 0.568\,9418^{[0]}$ [27] (0.568 9417)
2	0.5	$0.605\,40 < E_g < 0.605\,71^{[0]}$ [27] (0.605 5539)
2	1	$0.6246 < E_g < 0.6431^{[0]}$ [27] (0.633 078)
2	2	$0.5258 < E_g < 0.8023^{[0]}$ [29] (0.656 869)

^a P_{\max} .

[1] One missing moment formulation, equation (4.3).

[0] Zero missing moment formulation, equation (4.4).

AB Auberson and Boissiere (1983).

for $z \in [-1, 1]$. Note that the singularities at $z^2 = 1$ correspond to the essential singularities $\exp(\pm O(z^2/(1 - z^2)))$ for the unphysical and physical solutions, respectively. Because of these essential singularities, the Hausdorff moments $\sigma(p) \equiv \int_{-1}^1 z^p \Psi(z) dz$ are infinite and finite for unphysical and physical $\Psi(z)$ configurations, respectively. For the symmetric ground state, the associated moment equation is

$$\begin{aligned}
 [(2p+5)(2p+7)]h(p+3) &= [(2p+5)(8p+15) \pm (2/\alpha)(\alpha g)^{-2}]h(p+2) - [3(2p+3)(4p+5) \\
 &\quad - (\alpha g)^{-2} - 2E/\alpha g]h(p+1) + [(2p+1)(8p+5) \\
 &\quad - 2E/\alpha g]h(p) - 2p(2p-1)h(p-1)
 \end{aligned}
 \tag{4.6}$$

where $h(p) \equiv \sigma(2p)$. All references in table 5 to '[h]' refer to the numerical implementation of the above, except for the case $\alpha = 2$ which is discussed below. Observe that the

unconstrained missing moment order for equation (4.6) is 2. Generally, better bounds are obtained for the Hausdorff formulation (since it involves mapping the original singularity to infinity) than for the zero missing moment formulation, as reflected by the numerical results in the cited table.

Table 5. E_g bounds for potential $\frac{1}{2}x^2 - gx^4/(1 + \alpha gx^2)$.

α	g	E_g bounds
2	0.01	$0.492\ 610\ 46 < E_g < 0.492\ 610\ 51^{[0]}$ [28] ^a
2	0.1	$0.434\ 583\ 28 < E_g < 0.434\ 583\ 31^{[h]}$ [20] $0.380 < E_g < 0.523^{[0]}$ [25] (0.434 583 30) ^{AB}
2	0.2	$0.383\ 654 < E_g < 0.383\ 660^{[h]}$ [19] $0.1 < E_g < 1.26^{[0]}$ [28] (0.383 6567)
2	0.5	$0.2803 < E_g < 0.2829^{[h]}$ [20] (0.281 05)
2	1	$0.175 < E_g < 0.224^{[h]}$ [21] (0.190)
2.5	0.1	$0.441\ 2758 < E_g < 0.441\ 2766^{[h]}$ [20] ^a (0.441 2762)
2.5	0.2	$0.403\ 6618 < E_g < 0.403\ 7374^{[h]}$ [20] $0.4026 < E_g < 0.4047^{[0]}$ [28] (0.403 7167)
2.5	0.5	$0.3417 < E_g < 0.3486^{[h]}$ [19] (0.344 03)
2.5	1	$0.293 < E_g < 0.365^{[h]}$ (0.303)
3	.01	$0.492\ 788\ 132\ 867\ 68 < E_g < 0.492\ 788\ 132\ 867\ 71^{[0]}$ [26]
3	0.1	$0.446\ 2748 < E_g < 0.446\ 277\ 50^{[h]}$ [19] $0.446\ 267 < E_g < 0.446\ 282^{[0]}$ [28] (0.446 2756)

^a P_{max} .

^[0] Zero missing moment formulation, equation (4.4).

^[h] Hausdorff formulation, equations (4.6), and (4.8) for $\alpha = 2$.

^{AB} Auberson and Boissiere (1983).

The limit $\alpha \rightarrow 2$ is singular for the potential $V(x) = \frac{1}{2}x^2 - gx^4/(1 + \alpha gx^2)$, because the overall asymptotic behaviour goes from $(\frac{1}{2} - \alpha^{-1})x^2$ to $1/4g$. The preceding Hausdorff transformation results in the equation

$$\left[(1 - z^2)^3 \frac{d^2\Psi}{dz^2} - 3z(1 - z^2)^2 \frac{d\Psi}{dz} \right] - \frac{z^2}{(2g)^2} \Psi(z) = \frac{-E}{g} \Psi(z) \tag{4.7}$$

for $z \in [-1, 1]$. The resulting moment equation (involving only one unconstrained missing moment, $h(1)$) is

$$\begin{aligned} [(2p + 3)(2p + 5)]h(p + 2) &= [6(p + 1)(2p + 3) - (2g)^{-2}]h(p + 1) + [(E/g) \\ &- 3(2p + 1)^2]h(p) + 2p(2p - 1)h(p - 1). \end{aligned} \tag{4.8}$$

The ensuing analysis for $\alpha = 2$ is given in table 5.

5. The $-Z/(|x| + \alpha)$ potential

Our final potential problem is that corresponding to a one-dimensional, regulated, Coulomb potential:

$$-\frac{d^2\Psi}{dx^2} + \frac{-Z}{|x| + \alpha}\Psi(x) = E\Psi(x) \quad (5.1)$$

for $Z \equiv 1$. This problem, well studied by Loudon (1959) and Haines and Roberts (1969), simulates the slowly converging ground-state eigenenergy bounds encountered in the superstrong magnetic field limit, $\alpha \rightarrow 0$, for the quadratic Zeeman effect. We examine different methods designed to increase the convergence rate of these bounds.

The basic problem is to determine the ground-state eigenenergy for equation (5.1). The desired ground-state configuration is symmetric, with $\Psi'(0) \equiv 0$. The ground-state energy is clearly negative, thus we take $E \equiv -\epsilon$.

5.1. Zero missing moment formulation

Our first approach will be to use the results of Handy and Lee (1991), as summarized in the context of equation (2.7), to transform the system into one with as few missing moments as possible. The dominant asymptotic behaviour for the unphysical and physical configurations is determined by a zeroth-order JWKB analysis, or $\Psi(x) \rightarrow \exp(\pm\sqrt{\epsilon}x)$, for $x \rightarrow \infty$. Taking

$$\Phi(x) \equiv \Psi(x) \exp(-\sqrt{\epsilon}x) \quad \text{for } x \geq 0 \quad (5.2)$$

yields a new representation satisfying the differential equation

$$\frac{d^2\Phi}{dx^2} + 2\sqrt{\epsilon}\frac{d\Phi}{dx} + \frac{1}{x + \alpha}\Phi(x) = 0 \quad x \geq 0. \quad (5.3)$$

The corresponding Stieltjes moment equation (making use of the relation $\Phi'(0) = -\sqrt{\epsilon}\Phi(0)$) is

$$\begin{aligned} [2(p+1)\sqrt{\epsilon} - 1]u(p) &= [[1 - \alpha\sqrt{\epsilon}]\delta_{p,0} + \alpha\delta_{p,1}]\Phi(0) \\ &+ p[p+1 - 2\alpha\sqrt{\epsilon}]u(p-1) + \alpha p(p-1)u(p-2) \quad p \geq 0. \end{aligned} \quad (5.4)$$

Upon imposing the normalization $\Phi(0) \equiv 1$, the above equation becomes a zero missing moment problem. The zeroth moment is then $u(0) = (\alpha\sqrt{\epsilon} - 1)/(1 - 2\sqrt{\epsilon})$ and must be positive. The latter condition yields the bounds: $\frac{1}{2} \leq \sqrt{\epsilon} \leq \frac{1}{\alpha}$, if $\alpha \leq 2$; or $\frac{1}{\alpha} \leq \sqrt{\epsilon} \leq \frac{1}{2}$, if $\alpha \geq 2$. Note then that for $\alpha = 2$ the energy becomes $E_{\text{gr}} = -\epsilon = -0.25$. The results in table 6 are consistent with this (i.e. results referenced by ^[10]).

5.2. Hausdorff formulation I

Clearly, the preceding results are not too good, particularly for small α . As in the previous potential problem, we try to improve things by adopting a Hausdorff formulation in which the pole $x = -\alpha$ is mapped to infinity. This can be accomplished through the transformation $y = x/(x + \alpha)$, for $x \in [0, \infty)$; therefore, $y \in [0, 1)$. This transformation will not be done with respect to the Ψ representation, but with respect to a new representation:

$$\Phi_-(x) \equiv \Psi(x) \exp(+\sqrt{\epsilon}|x|). \quad (5.5)$$

Table 6. $-E_g$ bounds for potential $-1/(|x| + \alpha)$.

α	$-E_g$ bounds
1.96	$0.254\,059 < -E_g < 0.254\,085^{[0]} [12]^a$
1	$0.429\,910\,60 < -E_g < 0.429\,910\,95^{[b_2]} [30]$ $0.429\,89 < -E_g < 0.429\,93^{[0]} [30]$ $0.428\,76 < -E_g < 0.430\,86^{[h_1]} [24]$
0.1	$2.123 < -E_g < 2.132^{[b_2]} [30]$ $1.9881 < -E_g < 2.2201^{[h_1]} [24]$ $0.25 < -E_g < 3.25^{[0]} [30]$
0.01	$6.751 < -E_g < 8.551^{[b_2]} [30]$

^a P_{max} .

^[0] Zero missing moment formulation, equation (5.4).

^[h₁] Hausdorff formulation, equation (5.9).

^[b₂] Hausdorff formulation, equation (5.12).

The above representation transforms physical and unphysical Ψ configurations into unphysical (infinite moment) Φ configurations, with respect to the x -domain, therefore becoming unsuitable for implementing a moment analysis (Handy and Lee 1991). That is, the physical Ψ configurations become asymptotically finite Φ_- configurations (i.e. $\Phi_-(x \rightarrow \pm\infty) = \text{finite}$); while the unphysical Ψ configurations become asymptotically infinite Φ_- configurations (i.e. $\Phi_-(x = \pm\infty) = \text{infinite}$, for either or both $x = \pm\infty$).

However, these asymptotic properties become suitable for a moment's analysis if we work in the y -domain: $\Upsilon(y) \equiv \Psi(\alpha y/(1 - y)) \exp(+\sqrt{\epsilon}\alpha y/(1 - y))$. An immediate result is that physical and unphysical $\Upsilon(y)$ configurations have finite and infinite Hausdorff moments, respectively.

It is preferable to work within the domain $w \equiv 1 - y$, for $y \in [0, 1]$. The corresponding ($\Omega(w) \equiv \Upsilon(1 - w)$) differential equation is

$$w \frac{d}{dw} w^2 \frac{d\Omega}{dw} + 2\alpha\sqrt{\epsilon}w \frac{d\Omega}{dw} + \alpha\Omega(w) = 0 \tag{5.6}$$

for $w \in [0, 1]$. Before giving the relevant Hausdorff moment equation we make note of several important integral and boundary value relations. First,

$$\int_0^1 w^p \Omega'(w) dw = \Omega(1) - \delta_{p,0}\Omega(0) - pu(p - 1) \tag{5.7}$$

and

$$\int_0^1 w^p \frac{d}{dw} w^2 \frac{d\Omega}{dw} dw = \Omega'(1) - \delta_{p+2,0}\Omega'(0) - p\Omega(1) + p\delta_{p+1,0}\Omega(0) + p(p + 1)u(p). \tag{5.8}$$

Second, for the physical configurations: $\Omega(w = 0) \equiv \Upsilon(y = 1) \equiv \Phi_-(x = \infty) = \text{finite}$, and $\Omega(w = 1) \equiv \Upsilon(y = 0) \equiv \Phi_-(x = 0) \equiv \Psi(0) \neq 0$. Also, $\Phi'_-(x) \equiv -\frac{1}{\alpha}w^2\Omega'(w)$. Combining this with

$$\Phi'_-(x) \equiv \exp(\sqrt{\epsilon}x)[\sqrt{\epsilon}\Psi(x) + \Psi'(x)]$$

yields

$$\Phi'_-(x = 0) \equiv -(1/\alpha)\Omega'(w = 1) \equiv \sqrt{\epsilon}\Psi(x = 0) \neq 0$$

and $\Phi'_-(x = \infty) = \text{finite constant} = -(1/\alpha)0^2\Omega'(w = 0)$. The latter is important because in the process of generating the appropriate Hausdorff moment equation, expressions of the form $w^{p+3}\Omega'(w)$, for $w = 0$, are encountered. These are then necessarily zero. Finally, the desired Hausdorff moment equation is

$$(p + 2)(p + 1)u(p + 1) = \alpha[2\sqrt{\epsilon}(p + 1) - 1]u(p) + [p + 1 - \alpha\sqrt{\epsilon}]\Psi(0) \quad \text{for } p \geq 0 \tag{5.9}$$

where $u(p) \equiv \int_0^1 w^p \Omega(w) dw$. Note that both $u(0)$ and $\Psi(0)$ are arbitrary initialization variables (missing moments), that can be normalized to unity: $u(0) + \Psi(0) = 1$. The results of this analysis are given in table 6, refer to the numerical entries referenced by [h₁].

5.3. Hausdorff formulation II: moments of negative power

There is a clear improvement in the bounds obtained through the above Hausdorff reformulation, particularly for the case $\alpha = 0.1$. We can even do better by adopting the transformation in equation (5.2), but work with inverse moments instead! Specifically, we use the same coordinate transformations as before ($y = x/(x + \alpha)$, $w = 1 - y$) to define

$$\Xi(w) \equiv \Psi\left(\alpha \frac{(1-w)}{w}\right) \exp\left(-\sqrt{\epsilon}\alpha \frac{(1-w)}{w}\right) \quad \text{for } w \in [0, 1). \tag{5.10}$$

The representation in equation (5.2) will result in physical solutions exponentially going to zero as $x \rightarrow \infty$ or $w \rightarrow 0$. Likewise, unphysical solutions will go to a finite constant, asymptotically ($\Xi(0) = \text{finite}$). Note that, in both cases, at $w = 1$ the physical and unphysical configurations are finite. These facts lead to the observation that the inverse moments $v(p) \equiv \int_0^1 w^{-p} \Xi(w) dw$, for $p \geq 1$, will be finite, for the physical case, and infinite, for the unphysical case. This is precisely what must be satisfied in order that a moment's analysis be implementable (Handy and Lee 1991)!

The corresponding differential equation is

$$w \frac{d}{dw} w^2 \frac{d\Xi}{dw} - 2\alpha\sqrt{\epsilon}w \frac{d\Xi}{dw} + \alpha\Xi(w) = 0 \tag{5.11}$$

where the associated moment equation is

$$\alpha[2p\sqrt{\epsilon} - 1]v(p + 1) = p(p - 1)v(p) + [p - \alpha\sqrt{\epsilon}]\Psi(0) \tag{5.12}$$

for $p \geq 0$. Note that

$$\Phi(x) \equiv \exp(-\sqrt{\epsilon}|x|)\Psi(x) \quad \Phi'(x) = -\sqrt{\epsilon}\Phi(x) + \exp(-\sqrt{\epsilon}x)\Psi'(x)$$

and $\Phi'(x) = -\alpha^{-1}w^2\Xi'(w)$ (the latter two for positive x), where $\Psi'(0) \equiv 0$ is our boundary condition. Also observe that $v(0)$ does not contribute in the recursion relation. Instead, equation (5.12) corresponds to, effectively, a zero missing moment problem.

Although in this paper we have not dealt explicitly with the linear programming structure of the *cutting method*, as discussed in detail in the cited references, we do indicate here the nature of the linear inequalities considered in using equation (5.12). Specifically, we must work with the relations $\int_0^1 K_\sigma(w) [\sum_{i=0}^I C_i w^{-i}]^2 w^{-1} \Xi(w) \geq 0$, for arbitrary C s and $I \geq 0$; where $\sigma = 0, 1$ and $K_0(w) \equiv 1$ while $K_1(w) \equiv w^{-1} - 1$. The w^{-1} factor (in the integral expression) is critical, otherwise inappropriate $v(0)$ moments would appear. Utilizing these relations in the manner outlined in the cited references leads to the results shown in table 6.

6. Summary

We have applied the eigenvalue moment method to various important one-dimensional Schrödinger potential problems. The results show the effectiveness of this approach, when combined with appropriate transformations, in generating tight bounds for the ground-state energy. Extension to excited states is possible through the methods developed by Handy and Lee (1991). All numerical results (except those for the regulated one-dimensional Bohr atom) were done in double precision on an IBM RISC 6000/560. The higher-order regulated Bohr atom calculations were done in double precision on the CRAY.

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