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The perturbed two-dimensional oscillator: eigenvalues and infinite-field limits via continued fractions, renormalised perturbation theory and moment methods

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Abstract. We employ two independent methods to obtain consistent and accurate values of eigenvalues $E(\lambda)$ of the perturbed two-dimensional oscillator Hamiltonian, $H = H^{(0)} + \lambda x^2 y^2$: (i) continued-fraction representations of the Rayleigh-Schrödinger perturbation series to large order, as well as a renormalised version of perturbation theory, and (ii) a method of moments based on the positivity properties of the factorised wavefunction. The latter generates converging upper and lower bounds to $E(\lambda)$. The two methods are also used to obtain estimates for the eigenvalues $F^{(0)}$ of the infinite-field limit Hamiltonian, $H_\infty = p_x^2 + p_y^2 + x^2 y^2$.

Introduction

In this paper we examine the eigenvalues $E(\lambda)$ of the following two-dimensional perturbed oscillator Hamiltonian:

$$\begin{aligned} H &= -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + x^2 + y^2 + \lambda x^2 y^2 \\ &= H^{(0)} + \lambda x^2 y^2 \qquad (1.1) \end{aligned}$$

a special case of the more general family of problems defined by

$$H = p_x^2 + p_y^2 + Ax^2 + By^2 + Cx^2y^2 + Dx^4 + Fy^4. \qquad (1.2)$$

Hamiltonians of the above form have received attention from the viewpoint of perturbation theory and quantum field theory (Banks *et al* 1973), molecular spectroscopy (Percival and Pomphrey 1976) as well as dynamical systems theory (Pullen and Edmonds 1981). Various methods of obtaining good estimates of the eigenvalues of such Hamiltonians have been devised, including inner product perturbation theory (Killingbeck and Jones 1986) and a modified perturbation theory (Fernandez and Castro 1986).

Here, we focus on two independent methods to obtain consistent and accurate values of $E(\lambda)$ over the infinite range $0 < \lambda < \infty$ of the coupling constant: (i) a renormalised version of traditional Rayleigh-Schrödinger perturbation theory (RSPT), and (ii) a method of moments based on the positivity properties of the (factorised)

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wavefunction. In addition, we obtain accurate estimates for the eigenvalues $F^{(0)}$ of the 'infinite-field' Hamiltonian associated with (1.1):

$$\hat{H}_\infty = p_x^2 + p_y^2 + x^2y^2. \tag{1.3}$$

The importance of these eigenvalues arises as follows: a (unitary) scaling transformation $x \to \alpha x$, $y \to \alpha y$, $\alpha > 0$, of the Hamiltonian in (1.1) shows that its eigenvalues $E(\lambda)$ admit the asymptotic expansion

$$E(\lambda) \sim \lambda^{1/3} \sum_{n=0}^{\infty} F^{(n)} \lambda^{-2/3} \qquad \lambda \to \infty \tag{1.4}$$

i.e. the eigenvalues $F^{(0)}$ of (1.3) appear as the leading-order coefficients in (1.4). To estimate $F^{(0)}$, the moment method may be applied directly to the Hamiltonian in (1.3). As far as RSPT is concerned with the infinite-field problem, we first demonstrate that the RS perturbation series is divergent but asymptotic to $E(\lambda)$ and Stieltjes, admitting a Stieltjes-type continued-fraction (CF) expansion whose coefficients c_n grow linearly with n. A knowledge of this latter behaviour allows the construction of converging estimates to $F^{(0)}$ in terms of the c_n. Even more effective in this context, however, is a 'renormalisation' method which effectively transforms the RS series into a new series which is summable to $F^{(0)}$. Let us finally mention that our discussions will be restricted to the ground state. The perturbation methods apply directly to excited states. The moment method is also applicable, but with some minor modifications.

2. Rayleigh–Schrödinger perturbation theory (RSPT) and continued fractions (CF) at large order

Let us denote the RS expansion for the ground state of (1.1) as

$$E(\lambda) = \sum_{n=0}^{\infty} E^{(n)} \lambda^n = E^{(0)} + \lambda \Delta E(\lambda) \tag{2.1}$$

where $E^{(0)} = 2$, $E^{(1)} = \frac{1}{4}$. (The first ten coefficients are tabulated in Killingbeck and Jones (1986).) A numerical asymptotic analysis of the $E^{(n)}$ reveals that

$$E^{(n)} \sim (-1)^{n+1} A(\tfrac{3}{8})^n \Gamma(n + \tfrac{1}{2}) \qquad n \to \infty \tag{2.2}$$

where $A \simeq 0.780\,750\,50$. This is consistent with the results of Banks *et al* (1973), who analysed the large-order behaviour of RS expansions associated with (1.2). The large-order formulae are calculated from WKB tunnelling estimates in the limit $\lambda \to 0^-$.

We now consider the continued-fraction (CF) representation of the series in (2.1), having the form

$$E(\lambda) = E^{(0)} + \lambda C(\lambda) \tag{2.3}$$

where

$$C(\lambda) = \cfrac{c_1}{1 + \cfrac{c_2\lambda}{1 + \cfrac{c_3\lambda}{1 + \ddots}}}\,. \tag{2.4}$$

A few major properties of continued fractions are given below. Comprehensive treatments may be found in the books by Baker (1975), Baker and Graves-Morris (1980), Henrici (1977) and Jones and Thron (1980). The CF in (2.4) is non-terminating (unless $E(\lambda)$ is rational). By setting $c_{n+1}=0$, we produce the nth convergent $w_n(\lambda)$ to $C(\lambda)$, which may be written as a rational function:

$$w_n(\lambda)=\cfrac{c_1}{1+\cfrac{c_2\lambda}{1+\cfrac{c_3\lambda}{1+\ddots_{\,1+c_n\lambda}}}}=\frac{A_n(\lambda)}{B_n(\lambda)}. \tag{2.5}$$

The polynomials $A_n(\lambda)$ and $B_n(\lambda)$ satisfy the recurrence relations

$$\begin{aligned}A_n(\lambda)&=A_{n-1}(\lambda)+c_n\lambda A_{n-2}(\lambda)\\ B_n(\lambda)&=B_{n-1}(\lambda)+c_n\lambda B_{n-2}(\lambda)\qquad n=2,3,4,\ldots\end{aligned} \tag{2.6}$$

with initial values $A_0=0$, $B_0=1$, $A_1=c_1$, $B_1=1$. An induction argument shows that $L=\deg\{A_n(\lambda)\}=[(n-1)/2]$ and $M=\deg\{B_n(\lambda)\}=[n/2]$ where $[x]=$ integer part of x. The CF representation of the RS perturbation series in (2.3) satisfies the relations

$$\Delta E(\lambda)-w_n(\lambda)=O(\lambda^{n+1})\qquad n=1,2,3,\ldots. \tag{2.7}$$

From (2.5), these relations are equivalent to

$$\Delta E(\lambda)-A_n(\lambda)/B_n(\lambda)=O(\lambda^{L+M+1}) \tag{2.8}$$

which is the condition defining the unique $[L, M]$ Padé approximants (Baker 1975)

$$[L, M]=\sum_{i=0}^{L}p_iz^i\left(1+\sum_{j=0}^{M}q_jz^j\right)^{-1} \tag{2.9}$$

to the $E(\lambda)$ series.

The particular CF representations in (2.3) and (2.4) are chosen since many RS expansions of the form (2.1) are negative Stieltjes starting at $E^{(1)}$ (Simon 1970). It then follows that $C(\lambda)$ is an S fraction, i.e. that $c_n>0$, $n\geqslant 1$. The convergents $w_{2N}(\lambda)=[N-1, N](\lambda)$ and $w_{2N+1}(\lambda)=[N, N](\lambda)$ yield, respectively, lower and upper bounds to $E(\lambda)$ on the positive real line. These bounds converge to $E(\lambda)$ as $N\to\infty$ if the moment problem is determinate. A sufficient condition for determinacy is that the RS coefficients $E^{(n)}$ grow no faster than $(2n)!$ as $n\to\infty$, or that the CF coefficients grow no faster than n^2 (Henrici 1977).

Using the quotient-difference (QD) algorithm (Henrici 1977, see also Vrscay and Cizek 1986), the first 100 coefficients c_n of the ground-state representation have been calculated accurately. A numerical analysis, based on the effective use of the Thiele CF interpolation methods (Baker 1975) as well as a modified Neville scheme (Bender and Orszag 1978), indicates that the c_n behave asymptotically as

$$c_n\sim\tfrac{3}{16}n+(-1)^n\tfrac{1}{32}+o(1)\qquad n\to\infty. \tag{2.10}$$

The observed positivity of the c_n, indicating that $C(\lambda)$ is an S fraction, strongly suggests that the ground-state RS expansion in (2.3) is Stieltjes. The latter property has never been rigorously proved for two-dimensional coupled-oscillator problems although it is generally believed to be true. The relation between the asymptotic behaviour in (2.2) and (2.10) is in accordance with a general result relating the large-n behaviour of Stieltjes coefficients to their CF counterparts (Vrscay and Cizek 1986): if the $E^{(n)}$ are coefficients of a (negative) series of Stieltjes, and

$$E^{(n)}\sim(-1)^{n+1}A\Gamma(pn+a)B^n\qquad \text{as } n\to\infty$$

then

$$c_n \sim n^p \qquad \text{as } n \to \infty. \tag{2.11}$$

For the special case $p = 1$, then the following behaviour is often found:

$$c_n \sim \tfrac{1}{2}Bn + A^{(i)} + R_n^{(i)} \qquad i = \begin{cases} 1 & n \text{ even} \\ 2 & n \text{ odd} \end{cases} \tag{2.12}$$

where the $A^{(i)}$ are constants and $R_n^{(i)} = o(1)$ as $n \to \infty$. When the above behaviour exists, then a further intimate relation between the c_n asymptotics and $E(\lambda)$ is found: if

$$E(\lambda) \sim F^{(0)}\lambda^{\alpha} \qquad |\lambda| \to \infty \tag{2.13}$$

then

$$\alpha = \tfrac{1}{2} - \Delta A / B \qquad \Delta A \equiv A^{(1)} - A^{(2)}. \tag{2.14}$$

From (2.10), $A^{(1)} = -A^{(2)} = \frac{1}{32}$ and $B = \frac{3}{8}$ which implies that $\alpha = \frac{1}{3}$, in accordance with (1.4).

The result in (2.14) is obtained by replacing the infinite tail of the CF in (2.4) by 'approximate tails', i.e.

$$C(\lambda) \simeq \bar{w}_N(\lambda) \equiv \cfrac{c_1}{1 + \cfrac{c_2\lambda}{1 + \ddots \, 1 + c_{N-1}\lambda g_N(\lambda)}} \tag{2.15}$$

where

$$g_N(\lambda) = \cfrac{1}{1 + \cfrac{\bar{c}_N\lambda}{1 + \ddots}} \tag{2.16}$$

and

$$\bar{c}_n = \tfrac{1}{2}Bn + A^{(i)} \qquad n \geqslant N. \tag{2.17}$$

In other words, the asymptotic terms $R_n^{(i)}$ in (2.12) have been dropped from the CF coefficients in the 'tail'. This truncation procedure produces two sequences $\{\bar{w}_{N,\text{even}}\}$, $\{\bar{w}_{N,\text{odd}}\}$ which converge uniformly to $C(\lambda)$ in the limit $N \to \infty$ over compact subsets of the cut plane $|\arg(\lambda)| < \pi$. The new 'tail' functions $g_N(\lambda)$ may be written as ratios of contiguous Kummer confluent hypergeometric functions (details are given in Vrscay and Cizek (1986)). As a result, an asymptotic expansion of $g_N(\lambda)$ as $\lambda \to \infty$ may be determined. The 'finite' truncations of (2.15) are then written in terms of the partial numerators and denominators A_n and B_n of (2.6), i.e.

$$\bar{w}_N(\lambda) = \frac{A_{N-1}(\lambda) + \bar{c}_{N-1}\lambda g_N(\lambda) A_{N-2}(\lambda)}{B_{N-1}(\lambda) + \bar{c}_{N-1}\lambda g_N(\lambda) B_{N-2}(\lambda)}. \tag{2.18}$$

The dominant asymptotic behaviour of (2.18) is found to be

$$\bar{w}_N(\lambda) = W_N \lambda^{\alpha - 1} \qquad \lambda \to \infty \tag{2.19}$$

where α has been defined in (2.14), and the W_N are constants. (Note that substitution of this result into (2.3) yields the correct infinite-field behaviour (2.13).) The two sets of leading coefficients of (2.19) for the cases N even and odd are given by

$$W_{2n-1}=\frac{c_1c_3\ldots c_{2n-3}}{c_2c_4\ldots c_{2n-2}}c_{2n-1}\frac{\Gamma(\frac{1}{2}-\Delta A/B)\Gamma(n+A^{(1)}/B)}{\Gamma(\frac{1}{2}+\Delta A/B)\Gamma(n+\frac{1}{2}+A^{(2)}/B)}B^{-(1/2+\Delta A/B)} \tag{2.20a}$$

$$W_{2n}=\frac{c_1c_3\ldots c_{2n-1}}{c_2c_4\ldots c_{2n}}\frac{\Gamma(\frac{1}{2}-\Delta A/B)\Gamma(n+1+A^{(1)}/B)}{\Gamma(\frac{1}{2}+\Delta A/B)\Gamma(n+\frac{1}{2}+A^{(2)}/B)}B^{(1/2-\Delta A/B)}. \tag{2.20b}$$

Uniform convergence of the truncations $\tilde{w}_N(z)$ to $C(z)$ implies that $W_N\to F^{(0)}$ as $N\to\infty$. Note that

$$\frac{W_{2n}}{W_{2n-1}}=\frac{B\Gamma(n+1+A^{(1)}/B)}{c_{2n}\Gamma(n+A^{(1)}/B)}$$

$$=\frac{Bn+A^{(1)}}{c_{2n}}\to 1 \qquad \text{as } n\to\infty \tag{2.21}$$

where the limit follows from the asymptotic behaviour of the c_n in (2.12).

In table 1 are presented the numerical values of the estimates W_N for $N\leqslant 24$ along with an estimation of the limit of each sequence. The estimation was accomplished using the Thiele CF extrapolation method (Baker 1975).

Table 1. Approximations to the leading term coefficient $F^{(0)}$ in (2.6) as yielded by (2.20). The final entries represent estimates of the limits of these sequences, obtained from Thiele-Padé extrapolation.

n	W_{2n-1}	W_{2n}
1	1.028 135 7156	1.113 813 6919
2	1.135 653 1761	1.126 410 8308
3	1.132 483 7491	1.127 719 3700
4	1.130 263 3995	1.126 777 8702
5	1.128 122 4650	1.125 533 5363
6	1.126 386 5724	1.124 379 2923
7	1.124 973 9464	1.123 365 0819
8	1.123 811 0285	1.122 489 7087
9	1.122 842 3559	1.121 734 9575
10	1.122 024 3549	1.121 080 3416
11	1.121 324 3936	1.120 508 1485
12	1.120 718 2664	1.120 003 9438
13	1.120 187 7556	1.119 556 1217
14	1.119 718 9483	1.119 155 3935
15	1.119 401 0927	1.118 794 3225
16	1.118 925 7830	1.118 466 9260
17	1.118 586 3689	1.118 168 3562
18	1.118 277 5277	1.117 894 6542
19	1.117 994 9532	1.117 642 5611
20	1.117 735 1264	1.117 409 3736
21	1.117 495 1453	1.117 192 8317
22	1.117 272 5952	1.116 991 0326
23	1.117 065 4507	1.116 802 3628
24	1.116 871 9997	1.116 625 4448
∞	1.110 ± 0.002	1.110 ± 0.002

As stated earlier, the true convergents $w_n(\lambda)$ to $C(\lambda)$ provide upper and lower bounds to the Stieltjes function $E(\lambda)$ which converge to it as $n \to \infty$. This is the basis of the usual Padé or CF summability of the RS perturbation series. We postpone discussion of the application of this method to the next section, where it will be compared to a much more powerful summability method.

3. 'Renormalised' RS perturbation theory

In this section, we outline two possible methods of 'renormalising' standard RS perturbation expansions, effectively transforming a problem over the infinite coupling constant range $\lambda \in [0, \infty)$ into one over a finite range $\beta \in [0, 1)$, where β denotes the renormalisation parameter (Vrscay 1988). In both cases, the renormalisation is equivalent to a linear transformation of the original RS coefficients $E^{(n)}$, $n = 1, 2, \ldots$.

An immediate and attractive possibility of obtaining the infinite-field limit Hamiltonian H_∞ in (1.3) from our standard Hamiltonian in (1.1) is to construct the following 'renormalised' Hamiltonian:

$$\begin{aligned} H_R(\beta)\psi &= [p_x^2 + p_y^2 + x^2 + y^2 + \beta(x^2y^2 - x^2 - y^2)]\psi \\ &= G(\beta)\psi \end{aligned} \tag{3.1}$$

so that the eigenvalue $G(1)$ corresponds to the eigenvalue $F^{(0)}$ of H_∞ in (1.3). Clearly, $G(0) = E(0) = E^{(0)}$. We now assume a perturbation expansion to $G(\beta)$ of the form

$$G(\beta) = \sum_{n=0}^{\infty} G^{(n)}\beta^n. \tag{3.2}$$

If the coordinates in (3.1) are scaled as $x \to \tau^{1/2}x$, $y \to \tau^{1/2}y$, where $0 \leqslant \tau^2 = 1 - \beta \leqslant 1$, the eigenvalues of (3.1) and (1.1) are related as follows:

$$G(\beta) = (1-\beta)^{1/2}E(\beta(1-\beta)^{-3/2}). \tag{3.3}$$

This relation effectively defines a 'renormalisation map' on the positive real line, $R: \beta \in [0, 1) \to \lambda \in [0, \infty)$. If the RS expansions of $G(\beta)$ and $E(\lambda)$ are used formally in (3.3), along with the appropriate binomial expansion for $(1-\beta)^{-3/2}$, then a collection of like terms yields the relation

$$G^{(n)} = \sum_{k=0}^{n} \frac{\Gamma(k+n-\frac{1}{2})}{\Gamma(2k-\frac{1}{2})\Gamma(n-k+1)} E^{(k)}. \tag{3.4}$$

An asymptotic analysis of this relation shows that $G^{(n)} = O(E^{(n)})$ as $n \to \infty$. As in the case of one-dimensional problems, the Borel summability of the β series in (3.2) to $G(\beta)$ for $\beta \in [0, 1)$ can be established, since this problem differs very little from the usual multidimensional anharmonic oscillator problems, such as (1.2), which have been studied in detail (Simon 1971).

In table 2 are listed estimates of the ground-state eigenvalue $G(1) = F^{(0)}$ of the Hamiltonian H_∞ in (1.3). These estimates are obtained from convergents $w_n(\beta)$ to the continued-fraction representation of the renormalised β series in (3.2). This series is not rigorously Padé summable, so the estimates do not yield rigorous bounds to $G(1)$. Nevertheless, the diagonal Padé sequences generated by the convergents of CF representations to the renormalised β series demonstrate excellent convergence to limits which lie within the rigorous upper and lower bounds yielded by the moment method and in the next section.

Table 2. Estimates of the ground-state eigenvalue $G(1) = F^{(0)}$, of the infinite-field Hamiltonian H_∞ in (1.3), obtained from convergents $w_n(\beta)$ of the continued-fraction representation to the renormalised β series of (3.2).

n	$E^{(0)} + \beta w_n(\beta)$
1	1.25
5	1.116 4510
10	1.110 8372
20	1.108 3009
25	1.108 2650
26	1.108 2318
27	1.108 2537
28	1.108 2380
29	1.108 2445
30	1.108 2389

We may also employ the renormalisation equation (3.3) to accurately estimate ground-state eigenvalues $E(\lambda)$ over the entire range $0<\lambda<\infty$. The scaling transformations used to derive (3.3) are effectively inverted to give

$$E(\lambda) = \tau^{-1} G(1-\tau^2) \tag{3.5}$$

where τ is the root of the equation

$$\lambda\tau^3 + \tau^2 - 1 = 0. \tag{3.6}$$

Note that $\tau = 1$ ($\beta = 0$) when $\lambda = 0$ and $\tau \to 0$ ($\beta \to 1$) as $\lambda \to \infty$. For a given value of λ, $E(\lambda)$ is then calculated by (i) computing τ in (3.6) to a prescribed accuracy using, for example, the Newton–Raphson method (only one root lies in the interval (0, 1)), (ii) 'summing' the renormalised β series via Borel, Padé, etc, and (iii) computing $E(\lambda)$ from (3.5). The maximum error in $E(\lambda)$ will be incurred in the high-field limit $\lambda \to \infty$,

Table 3. Estimates of the ground-state eigenvalues $E(\lambda)$ to the Hamiltonian of (1.1), obtained from Padé approximants (continued-fraction convergents) to the (i) renormalised β series, (3.2) and (3.5), and (ii) usual RSPT λ series, (2.1). The entries in the table correspond to [14, 15] Padé approximants (w_{30}). The asterisk indicates that the [14, 14] Padé results (w_{29}) are obtained by replacing the last n digits by the n digits in parentheses. (The λ-series estimates $\lambda = 0.1$ are virtually identical to the β-series estimates and have not been included.)

λ	β series	λ series
0.1	2.024 138 321 415 731 606 391 632 59 (60)*	
0.5	2.108 213 779 698 540 (2)	2.108 213 779 698 4 (9)
1.0	1.195 918 085 201 (3)	2.195 918 084 5 (62)
2.0	2.339 566 210 4 (7)	2.339 565 9 (67)
3.0	2.458 376 909 (11)	2.458 37 (8)
4.0	2.561 626 587 (96)	2.561 6 (7)
5.0	2.653 909 81 (3)	2.653 8 (41)
10.0	3.019 178 1 (3)	3.017 (22)
100.0	5.460 99 (101)	4.78 (6.59)
1000.0	11.232 56 (61)	5.6 (37.5)
10000.0	23.946 3 (4)	5.7 (345.3)

i.e. $\beta = 1$, and is given by the error of $G(\beta = 1)$ in estimating $F^{(0)}$, since $E(\lambda) \sim F^{(0)}\lambda^{1/3}$ as $\lambda \to \infty$.

In table 3 we list some estimates of the ground-state eigenvalue $E(\lambda)$ for a range of λ values. For comparison, we include the results of direct Padé summation of the usual RS expansions.

4. Bounds for the ground-state eigenvalue by the moment method

In several recent works (Handy and Bessis 1985, Handy *et al* 1988ab, Bessis *et al* 1987) an eigenvalue moment method has been developed for generating rapidly converging exact bounds to ground-state energies of bosonic systems. These methods can be extended to excited states. However, we limit this discussion to an analysis of the ground state of our coupled oscillator problem. (Let us reiterate that the renormalised perturbation methods of the previous section, although providing excellent estimates of eigenvalues, do not establish rigorous bounds.)

The moment method is particularly effective for addressing strongly coupled singular perturbation problems. It exploits the unique non-negative character of the bosonic ground-state wavefunction $\psi(x)$ (Reed and Simon 1978) as well as its bounded asymptotic behaviour (Agmon 1983). The latter guarantees that the associated power moments:

$$\mu(n) = \int_R x^n \psi(x)\,\mathrm{d}x \tag{4.1}$$

where R denotes the appropriate (real) domain of integration, are finite. The combination of these two essential properties permits a transformation of the quantisation problem associated with the Schrödinger equation into a pure 'moment problem' (Shohat and Tamarkin 1963). An infinite hierarchy of moment constraints are defined which determine the allowed physical energy through rapidly converging bounds. The relevant details of the method are given in the references cited above. We illustrate briefly with the case of a one-dimensional Stieltjes moment problem, i.e. $R = [0, \infty)$, which is often encountered in Schrödinger eigenvalue problems. A necessary and sufficient condition for the sequence of positive numbers $\mu(n)$ to be moments of a non-negative distribution is that the Hankel–Hadamard determinants (Baker and Graves-Morris 1980), which are defined as

$$H(n, m) = \begin{vmatrix} \mu(n) & \mu(n+1) & \dots & \mu(n+m) \\ \mu(n+1) & \mu(n+2) & \dots & \mu(n+m+1) \\ \vdots & \vdots & & \vdots \\ \mu(n+m) & \mu(n+m+1) & \dots & \mu(n+2m) \end{vmatrix} \tag{4.2a}$$

satisfy the inequalities

$$H(0, m) > 0 \qquad H(1, m) > 0 \qquad m = 0, 1, 2, \dots . \tag{4.2b}$$

In the reformulated moment problem, the moments $\mu(n)$ will be functions of the unknown eigenvalue E. As m in these inequalities increases, i.e. as more moments are being incorporated, stronger constraints are being imposed on the intervals in which E can be found. These constraints manifest themselves as increasingly tighter upper and lower bounds to E.

The following moment analysis of the two-dimensional problem employs a special transformation. In order to emphasise its significance, as well as familiarise the reader with our notations, we first apply it to the trivial one-dimensional harmonic oscillator problem:

$$-\psi''+x^2\psi=E\psi. \tag{4.3}$$

The dominant asymptotic behaviour for physical and unphysical solutions to (4.3) is provided by the zeroth-order JWKB function:

$$\psi(x)\simeq\exp(\pm\tfrac{1}{2}x^2). \tag{4.4}$$

We now transform the original problem, (4.3), into one involving the function

$$\phi(x)=\exp(-\alpha x^2)\psi(x) \qquad -\tfrac{1}{2}<\alpha\leqslant\tfrac{1}{2}. \tag{4.5}$$

As in the ψ representation case, the ground state in the ϕ representation is unique, non-negative and has finite power moments $\mu(n)$. If $|\alpha|>\frac{1}{2}$, then unphysical ψ solutions, with infinite moments, will have associated bounded ϕ representations, with finite moments. In such cases, the moment method may not yield converging bounds to the ground-state energy.

In terms of the allowed α values, the transformed Schrödinger equation becomes

$$-(\phi''+4\alpha x\phi'+2\alpha\phi)+(1-4\alpha^2)x^2\phi=E\phi. \tag{4.6}$$

We now choose $\alpha=\frac{1}{2}$ to eliminate the last terms on the LHS. An integration of (4.6) by parts on the real line, with appropriate boundary conditions, shows that the Hamburger power moments of ϕ:

$$\mu(p)=\int_{-\infty}^{\infty}x^p\phi(x)\,\mathrm{d}x \tag{4.7}$$

satisfy the recursion relation

$$[E-1-2p]\mu(p)=-p(p-1)\mu(p-2). \tag{4.8}$$

Odd-order moments vanish since the ground-state wavefunction possess even parity. Through the simple change of variable, $y=x^2$, one can show that the even-order Hamburger moments are equal to Stieltjes moments of a suitably defined distribution, i.e.

$$\mu(2p)=u(p)=\int_0^{\infty}y^p\phi(y^{1/2})y^{-1/2}\,\mathrm{d}y. \tag{4.9}$$

The Stieltjes moments satisfy the recursion relation

$$(E-1-4p)u(p)=-2p(2p-1)u(p-1) \qquad p\geqslant 0. \tag{4.10}$$

The homogeneous nature of this moment equation shows that the 'initial condition', $u(0)$, is arbitrary. Keeping in mind that the physical ground-state wavefunction must be non-negative, we normalise the moments by setting $u(0)=1$. It then follows from (4.10) that the ground-state energy must be $E=1$.

Had the special transformation of (4.5) not been adopted, then a 'full moment method Hankel–Hadamard analysis' (Handy and Bessis 1985) would have been necessary. Bounds to the energy are also achieved with this formalism, but their rate of convergence is not as rapid. This is especially important for the problem to be discussed below.

The two-dimensional coupled-oscillator problem of (1.1) clearly exhibits a quartic anharmonic structure away from the x and y coordinate axes. Along these axes, it is harmonic in nature. A two-dimensional moment analysis may be performed directly on (1.1). However, a dramatic improvement in convergence can be achieved by transforming the wavefunction in a manner analogous to the one-dimensional problem, namely

$$\phi(x, y)=\psi(x, y) \exp[-\tfrac{1}{2}(x^2+y^2)]. \tag{4.11}$$

The ground-state wavefunction must satisfy the interchange and reflection symmetry conditions $\psi(x, y)=\psi(y, x)$ and $\psi(x, y)=\psi(-x, y)=\psi(x, -y)$, respectively. We define the two-dimensional Hamburger moments for this problem as

$$\mu(p, q)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} x^p y^q \phi(x, y)\, \mathrm{d}x\, \mathrm{d}y. \tag{4.12}$$

As in the one-dimensional case, moments with either p or q odd vanish. The non-zero moments are then equivalent to two-dimensional Stieltjes moments:

$$\mu(2p, 2q)=u(p, q)=\int_0^{\infty}\int_0^{\infty} x^p y^q \phi(x^{1/2}, y^{1/2}) x^{-1/2} y^{-1/2}\, \mathrm{d}x\, \mathrm{d}y. \tag{4.13}$$

Coordinate interchange symmetry yields $u(p, q)=u(q, p)$. The corresponding moment recursion relation for this problem is

$$\begin{aligned}\lambda u(p+1, q+1)={}&[E-2(2p+2q+1)]u(p, q)\\ &+[2p(2p-1)u(p-1, q)+2q(2q-1)u(p, q-1)].\end{aligned} \tag{4.14}$$

We designate the 'missing moments' to be the set $\{u(p, 0)\}$. Once the first $M+1$ of these are specified ($0 \leqslant p \leqslant M$), all the moments within the square $\{u(p, q) | 0 \leqslant p, q \leqslant M\}$ are determined. The homogeneous and linear dependence of the moments on the 'missing moments' can be represented by

$$u(p, q)=\sum_{k=0}^{M} M_E(p, q, k) u(k, 0) \qquad \text{for } 0 \leqslant p, q \leqslant M. \tag{4.15}$$

The normalisation prescription will be

$$\sum_{k=0}^{M} u(k, 0)=1 \tag{4.16}$$

which serves to constrain $u(0,0)$. The $M_E(p, q, k)$ are energy-dependent coefficients recursively obtainable from (4.14).

It has been established elsewhere (Handy *et al* 1988a, b) that the necessary and sufficient conditions for the moments in (4.14) to correspond to a non-negative function are given by the linear inequality constraints:

$$\begin{aligned}&\sum_{k=1}^{M} u(k, 0)\Big(-\sum_{\sigma_1, \sigma_2=1}^{D} C_{i_{\sigma_1}, j_{\sigma_1}} M_E(\tau+i_{\sigma_1}+i_{\sigma_2}, j_{\sigma_1}+j_{\sigma_2}, k) C_{i_{\sigma_2}, j_{\sigma_2}}\Big)\\ &\qquad < \sum_{\sigma_1, \sigma_2=1}^{D} [C_{i_{\sigma_1}, j_{\sigma_1}} M_E(\tau+i_{\sigma_1}+i_{\sigma_2}, j_{\sigma_1}+j_{\sigma_2}, 0) C_{i_{\sigma_2}, j_{\sigma_2}}]\end{aligned} \tag{4.17}$$

where $\tau=0,1$ and the $C_{i,j}$ are arbitrary. The coordinate sequence $(i_\sigma, j_\sigma)=(i, j)_\sigma$ is ordered as follows. First, a parameter $I \geqslant 0$ is chosen. We limit $(i, j)_\sigma$ to lie within the region $0 \leqslant i, j \leqslant I$. We take $(0,0)_{\sigma=1}$ and sequentially order the remaining $(I+1)^2-1$ points by varying i while keeping j fixed, i.e. $(0,0)_1, (1,0)_2, \ldots, (I,0)_{I+1}, (0,1)_{I+2}, \ldots$. From the nature of (4.17) it is clear that, for a given 'I', moments within the $[0, M]\times[0, M]$ square region will be required, where $M = 2I+1$ is the number of missing moments. The variable dimensionality, D, must satisfy the inequality $D \leqslant (I+1)$.

The linear programming 'cutting' methods developed in Handy *et al* (1988a, b) are used to analyse (4.17). The bounds obtained are cited in table 4. For purposes of comparison, table 5 presents the bounds obtained by moment methods without employing the transformation in (4.11). The improvements afforded by the transformation are easily seen. In both tables a rescaling of the moments, $u(p, q)s^{-(p+q)}$, was implemented in order to avoid large numbers. The parameter s was taken to satisfy $(2M)^2 s^{-3} = 1$, as motivated by considering the kinetic energy contribution to the moment equation in (4.14).

Table 4. Lower and upper bounds, $E^{(-)}$ and $E^{(+)}$, respectively, to the ground-state energy $E(\lambda)$ of (1.1), using the 'transformed' moment recursion relation, (4.14).

λ	I	D	$E^{(-)}$	$E^{(+)}$
1	1	4	2.1	2.3
	2	9	2.195	2.198
	3	16	2.195 91	2.195 95
	4	25	2.195 9178	2.195 9192
	5	30	2.195 9180	2.195 9182
10	1	4	2.6	4.7
	2	9	2.9	3.1
	3	16	3.014	3.027
	4	25	3.018 4	3.020 0
	5	36	3.019 1	3.019 3
	6	40	3.019 16	3.019 20
100	4	25	5.42	5.50
	5	36	5.45	5.47
	6	40	5.458	5.464
1000	4	25	10.8	11.4
	5	36	11.12	11.32
	6	49	11.20	11.26

Table 5. Lower and upper bounds, $E^{(-)}$ and $E^{(+)}$, respectively, to $E(\lambda)$ using moment relations associated with the 'untransformed' Schrödinger equation.

λ	I	D	$E^{(-)}$	$E^{(+)}$
1	4	25	2.188	2.214
	5	30	2.188	2.199
100	3	16	4.3	6.8
	4	25	5.1	5.8
	5	36	5.36	5.60
	6	46	5.42	5.50
	7	51	5.43	5.48

Table 6. Lower and upper bounds, $F^{(-)}$ and $F^{(+)}$, respectively, to the ground-state eigenvalue $F^{(0)}$ of the infinite-field Hamiltonian H_∞ in (1.3).

I	D	$F^{(-)}$	$F^{(+)}$
3	16	0.7	1.6
4	25	0.9	1.3
5	36	1.04	1.16
6	49	1.08	1.13

Finally, we apply the moment method to the infinite-field Hamiltonian, (1.3), to obtain bounds to the (ground-state) eigenvalue $F^{(0)}$. The missing moment structure, but not the equation, associated with the eigenvalue problem $H_\infty\psi = F\psi$ is identical to (4.14). In table 6 are presented bounds for $F^{(0)}$ yielded by this method. As mentioned in the previous section, the bounds bracket the estimates afforded by summability of the renormalised β series.

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