

Home Search Collections Journals About Contact us My IOPscience

Energy spectrum of the potential $V=ax^2+x^4$

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 1991 J. Phys. A: Math. Gen. 24 2731

(http://iopscience.iop.org/0305-4470/24/12/013)

View the table of contents for this issue, or go to the journal homepage for more

Download details: IP Address: 129.252.86.83 The article was downloaded on 01/06/2010 at 11:17

Please note that terms and conditions apply.

Energy spectrum of the potential $V = ax^2 + x^4$

S.C. Chhajlany, D.A. Letov* and V.N. Malnev*

Physics Department, Addis Ababa University, Box 32811, Addis Ababa, Ethiopia

Received 29 October 1990 in final form 20 February 1991

Abstract Suitable sequences of quasi-exactly solvable Hamiltonians are shown to provide stringent upper bounds to the energy eigenvalues of the bound state potential $V = av^2 + x^4$. Procedures to convert these bounds into even further improved energy estimates are developed. For the quartic anharmonic oscillator (a = 0) case a simple argument is provided to indicate that the conventional small-parameter energy expansion does not converge as a Taylor series. An accurate closed form parametrization of the entire quartic double well (a = 0) is satisfactorily recovered and for deep wells a useful expression is deduced for it empirically.

1. Introduction

Power law potentials, anharmonic oscillators and multiple-well potentials continue to remain a focus of attention in non-relativistic quantum mechanics. The real challenge is the lack of an adequately powerful universal approach for solving multiple-term recursion relations. Although enormous progress has been made over the years in our understanding of these problems, questions of a delicate nature inevitably arise in the process. The hardest amongst these often relate to the normalizability of the resulting wavefunctions and the existence of the assumed small-parameter expansions. A concise summary of the modern techniques for studying such potentials can be found in [1], which is also the basis of the present work.

The crucial problem of normalizability can be avoided by seeking manifestly normalizable solutions which, in practice, means polynomials with appropriate weights In fact, it is now known that many problems are quasi-exactly-solvable (QES), provided certain associated couplings are fine tuned, i.e suitably quantized A systematic study of QES Hamiltonians that owe their partial solvability to an underlying dynamical SL(2, R) symmetry has been provided by Turbiner [2] Hamiltonians with no apparent symmetry suddenly become expressible as functions of the generators of the SL(2, R)group upon the fine tuning of certain couplings A partial set of manifestly normalizable solutions then splits off from the rest and beco..ies tractable by elementary means Leach [3] has traced the origin of this circumstance to the factorizability of the Hamiltonian that reduces the problem to that of solving a Riccati equation. This approach is developed further in a series of papers by Leach and his co-workers [4] An independent approach to N-dimensional anharmonic oscillators that are QES is

Permanent address General Physics Department, Peoples Friendship University, Ordjonikidze Street, 3, Moscow, USSR

² Permanent address Physics Department, Kiev State University, Kiev, USSR

provided by Dutta and Willey [5]. To the best of our knowledge, Calogero [6] was the first to point out a general technique for constructing QFS Hamiltonians, albeit in the rather different context of singular perturbation theories and quantum catastrophes. The case of the sextic anharmonic oscillator was noted earlier by Singh *et al* [7].

Inspite of these vastly varying and exhaustive studies, or s problems have generally been considered to be of limited utility due to the discretization of couplings. In a recent paper [1], we have demonstrated that this should indeed not be so. A slightly different view of these problems shows that they are very rich in content. For many Hamiltonians there exists a sequence of QES Hamiltonians that approach them monotonically from above, providing thereby a string of upper bounds to the energy eigenvalues of the given problem The Hamiltonian of interest can thus be approached as closely as one wishes The importance of this last remark can be readily appreciated by recalling, for example, the case of the 1D quartic oscillator problem for which the extraction of the correct asymptotic factor creates difficulties of its own. Furthermore, questions of the type listed above simply cannot arise, since one deals only with manifestly normalizable solutions and the auxiliary couplings can be reduced at will Having done so, one has in hand an excellent approximate function that provides a further improved estimate of the eigenvalues sought, irrespective of the status of the attendant perturbation theories. The availability of a dense set of exact eigenvalues of the nearby Hamiltonians as a function of some auxiliary coupling naturally suggests elementary non-controversial graphical techniques that estimate energies even more precisely In fact, it turns out, as we shall see in the sequel, that the sequence of upper bounds in itself generates a sequence of tight lower bounds. The procedure thus becomes self contained

- This paper is primarily devoted to the following problems
- (1) the pure quartic potential $V = x^4$,
- (11) the quartic anharmonic potential $V = x^2 + \lambda x^4$, $\lambda > 0$,
- (iii) the quartic double-well potential $V = -ax^2 + x^4$, a > 0

To keep the work self contained, section 2 recapitulates the main steps of the framework of [1] and discusses three methods of its implementation in practice Section 3 considers the quartic potential. The ground state energy is computed extremely accurately and the result for the 100th excited state is also exhibited. The anharmonic potential $V = x^2 + \lambda x^4$ is discussed in section 4 and results for the cases of weak, medium and very strong anharmonicities are provided. Section 5 is devoted to the double-well potential $V = -ax^2 + x^4$. The splitting Δ between the ground and first excited states for deep double wells is computed. The last section is reserved for a summary of the results and various observations. Detailed applications and further development of our framework [1] is the main aim of the present study.

2. The theoretical framework

We outline our procedure [1] through the case of $V = bx^{\dagger}$, b > 0 To solve this problem we introduce the auxiliary potential

$$U_1 = bx^4 + cx^6 \qquad c > 0 \tag{21}$$

Using quartic scales the associated Schrodinger equation is

$$\Psi'' + (\varepsilon - \tau^4 - gx^6)\Psi = 0 \tag{2.2}$$

Fnergy spectrum of the potential
$$V = ax^2 + x^4$$
 2733

Let

$$\Psi = \exp\left(-\frac{\gamma}{2}x^2 - \frac{\sqrt{g}}{4}x^2\right)\iota(x)$$
(2.3)

The parameter γ will be specified shortly

From (2.2) we now have

$$\iota'' - 2(\sqrt{g} x^3 + \gamma x)\iota' + [\varepsilon - \gamma + (\gamma^2 - 3\sqrt{g})x^2 + (2\sqrt{g} y - 1)x^4]\upsilon = 0$$
 (24)

Choose

$$2\sqrt{g\gamma} = 1 \tag{2.5}$$

Setting $v = \sum a_n x^n$ we convert (2.4) into the three-step relation

$$(n+3)(n+4)a_{n+4} + [\varepsilon - \gamma(2n+5)]a_{n+2} + [\gamma^2 - \sqrt{g}(2n+3)]a_n = 0 \qquad (2.6)$$

For even-parity solutions $a_0 \neq 0$, $a_1 = 0$ and for odd-parity solutions $a_0 = 0$, $a_1 \neq 0$ Following the approach described first by Saxena and Varma [8] in relation to a three-term problem for the Killingbeck potential, we notice that (2.6) allows v(x) to be a polynomial of degree k provided

$$a_k \neq 0$$
 $a_{k-2} = a_{k+4} = 0$ (27)

with k = 2m or k = 2m + 1, m = 0, 1, 2, From (2.7) we immediately get

$$\gamma^2 = \sqrt{g}(2k+3) \tag{28}$$

so that

$$g = \left(\frac{1}{4(2k+3)}\right)^{2/3}$$
(2.9)

The condition $a_{k+2} = 0$ then provides an algebraic equation whose (m+1) roots determine the lowest (m+1) eigenvalues of one parity. The remainder of the solutions are not polynomials and will not concern us here. The origin of the (m+1) roots can be traced to the SL(2, R) symmetry connection of the problem [2] and is directly verifiable using the coefficient matrix approach of Saxena and Varma [8]

As k increases, so does the number of polynomial solutions. Remarkably, at the same time the tuned sextic coupling g decreases monotonically as per (2.9) and $U_1 \rightarrow V$. The energy eigenvalues $\varepsilon(g)$ then approach their quartic counterparts $\varepsilon(0)$ from above. This feature, shared by all problems to be discussed here, is the basis of our method. The condition $a_{k+2} = 0$ for any large finite k is easily solved numerically. This provides a sequence of tighter and tighter upper bounds $\varepsilon(g)$ to $\varepsilon(0)$. We shall find that $\varepsilon(g)$ are gentle monotonic functions of g that facilitate an easy translation of these bounds into remarkably accurate estimates of $\varepsilon(0)$ without recourse to the formal theory of analytic continuation.

The roots of the equation $a_{k+2} = 0$ can be computed in three different ways. The first is to convert it into the vanishing of a tridiagonal $(m+1) \times (m+1)$ determinant, which, for example, for even k(=2m) becomes

$$D(m+1) = 0 (2.10)$$

The non-vanishing elements of D(m+1) are

$$D_{qq} = \varepsilon - \gamma(4q-3) \qquad D_{qq} = 2q(2q-1)\delta_{q+1q}$$
$$D_{q|q} = [\gamma^2 - \sqrt{g}(4q-1)]\delta_{q|q+1} \qquad \text{where } 1 \le q, q' \le m+1$$

Equation (2^{-7}) can be solved as a matrix eigenvalue equation. For large k this is time consuming. Secondly, we can convert (2|10) into a recursion relation amongst determinants of the type

$$D(n+1) = [\epsilon - \gamma(4n+1)]D(n) - 2n(2n-1)[\gamma^2 - \sqrt{g}(4n-1)]D(n-1)$$
(2.11)

Setting D(-1) = 0 and normalizing D(0) suitably, the algebraic equation is easily solved. This is a very efficient method that exploits the fact that the *l*th root of D(m+1) lies lower than the *l*th root of D(m) and is not far from it for $m \ge 1$. Lastly, the recursion relation can itself be used repeatedly. We adopt the second method based on (2.11)

3. The potential $V = x^4$

A selection of results that represent a sequence of upper bounds for the first four levels and the 100th level is displayed in table 1. These are the exact energy eigenvalues of U_1 with g chosen as per (2.9).

Table 1. Upper bounds ε_i for five levels of the quartic potential $V = v^4$, ε_0 represents the ground state and ε_i the ith excited state. Exact energies are taken from [9]. For odd levels, the k-value is one more than that displayed in column 1. The residual sectic coupling is related to k through (2.9). All results have been rounded off at the sixth digit. With increasing k the convergence of ε_i to exact values is clearly seen.

k	£ .,	٤ 2	e 1 MI	۶ı	٠ 1
()				4 071 63	
10	1 084 98	7 721 46		3 902 33	12 1184
100	L 066-37	7 521 76	1107.04	3 826 12	11 7694
1 000	1 061 87	7 470 29	1042.34	3 805 53	11 6725
10.000	1 060 64	7 458 85	1025 76	3 800 94	11.6508
800.000	1.060.38	7 455 86	1021.25	3 799 74	11 6451
Exact	1 060 36	7 455 70	1020 99-	3 799 67	11 6447

· Taken from VKB

They bear out the claims made in the previous section As k increases, the auxiliary coupling g decreases and $\varepsilon(g)$ approaches $\varepsilon(0)$ from above

A comparison with the numerical results [9] brings out the anticipated fact that the bounds deviate from $\varepsilon(0)$ by essentially an order of g correction. Throughout the domain of polynomial solutions g < 0.2. Hence U_1 never really differs substantially from V. The corresponding wavefunctions thus provide a natural set of good substitutes for the unknown quartic functions. Using these to estimate $\langle H_{quartic} \rangle$ we obtain very much improved estimates of $\varepsilon(0)$. For the ground and first excited states, these are readily seen to be upper bounds. For the other states the same turns out to be true for reasons to be explained shortly.

Let us first get some qualitative feeling for the results At k = 0 ($g \approx 0.19$, v(x) = const) the ground state result is ~75% above the quartic ground state energy ε_0 while the improved boun is merely ~1% above. This is indeed gratifying At $k \sim 10$, the corrected estimate is about 01% higher and at $k \sim 100$, the corrected result is 1.060.55, compared with the numerical value of 1.060.36. This feature is typical of all levels. We

have checked it up to the 100th level. The first direct bound is about 7.5-8.5% higher. The corrected one is about 1% higher. The entire quartic spectrum can thus be bounded to roughly 1% using this elementary approach. This is seemingly puzzing. The higher the level the more one expects it to be perturbed by the residual sextic coupling. This is indeed so, but at the same time a compensating factor appears in that the higher the level the smaller is the residual g-value that gives rise to it first time. To sum up, all levels up to the 20th, at least, can be bounded to better than 1 part in about 20 000 at k = 200 i.e. via 100×100 determinants.

At higher k, this approach, although perfectly valid and straightforward, becomes tedious. There is an ever-increasing number of integrals to be evaluated numerically Happily, it can be replaced by an elementary graphical technique that accomplishes about the same results.

Consider, for example, the ground state energy $\varepsilon_0(g)$ Plot $\varepsilon_0(g)$ against g for $g \leq 0.2$ Any number of exact data points are available. The $\varepsilon - g$ curve is found to be a smooth monotonic curve with a very gentle departure from linearity that renders it concave down throughout Hence, every linear extrapolation using two points on the curve provides an upper bound to ε_0 The closer the two points to g = 0, the tighter is the bound. Taking the two points around $k \sim 8 \times 10^5$ (i.e. $g \sim 10^{-5}$) we find ε_0 (upper bound) $\sim 1.060\ 362\ 0909$. Compare this with standard result [9] $\varepsilon_0 = 1\ 060\ 362\ 09048$. Better agreement can be obtained by going to smaller g. The same holds for other levels Table 2 provides the improved bounds for the levels of table 1.

k	E _U	E ₁	£100	£	ε3
100 98	1 060 44	7 457 0		3 800 1	11 647 6
1 000 990	1 060 366	7 455 76	1021 9	3 799 69	11 644 9
10 000 9 000	1 060 362 7	7 455 701	1021 038	3 799 674	11 644 75
800 000 790 000	1 060 362 090 9	7 455 697 946	1020 9901	3 799 673 032	21 644 745 53
'Exact † 'Lower'	1 060 362 090 5 1 060 361 7	7 455 697 938 7 455 693 5	1020 . 99 ≖	3 799 673 029 3 799 671 2	11 644 745 51 11 644 737

Table 2. Improved upper bounds for the levels of table 1 based on the linear extrapolation scheme using two nearby k-values. The lower bounds are from the $\varepsilon - g^{\alpha}$ graph for $\alpha = 0.975$. The k-values for the odd levels equal the k + 1 values of column 1.

† Taken from [9]

Taken from WKB

Lower bounds obtained by plotting $\varepsilon(g)$ against g^{α} , $\alpha \le 0.98$ For $k \ge 100$ the entire curve is now marginally convex down A linear extrapolation thus gives lower bounds. For $\alpha = 0.975$, for example, we get the lower bound ε_0 (lower bound) $\approx 1.060.3617$. This bound too can be tightened if one so desires. Our method is thus self contained. The interval $0.98 < \alpha < 1$ is avoided as the curvature of the $\varepsilon - g^{\alpha}$ curve does not have a fixed sign throughout. Hence, the nature of the bound cannot be deduced.

To conclude this section we note that, given the information available, one can also deduce a number of interesting features of the energy spectrum of the auxiliary potential $U_1 = x^4 + gx^6$ for $0 \le g \le 0.2$ Firstly, for any value of g in the above range one has in hand good upper and lower bounds to the energies. Secondly, the levels themselves can be estimated to an excellent approximation Thirdly, useful knowledge of levels somewhat outside the range can be obtained. Lastly, it is also possible to gain some insight into the nature of the energy function near g = 0. We shall not enter into the details here.

4. The anharmonic potential $V = x^2 + \lambda x^4$

We introduce the auxiliary potential

$$U_2 = ax^2 + bx^4 + cx^6 \qquad c > 0. \tag{41}$$

Using oscillator units we have to solve the equation

$$\psi'' + (\varepsilon - x^2 - \lambda x^4 - gx^6)\psi = 0 \tag{42}$$

Proceeding exactly as in section 2, polynomial solutions of degree k obtain if

$$2\sqrt{g} \ \gamma = \lambda \tag{43}$$

$$\gamma^2 = 1 + \sqrt{g}(2k+3) \tag{4.4}$$

so that

$$\gamma^3 - \gamma = \frac{\lambda(2k+3)}{2}.$$
 (45)

As before, energy eigenvalues follow from the condition $a_{k+2} = 0$

Some results which represent improved bounds as per the linear extrapolation scheme are presented in table 3 and compared with the 'exact' results of Biswas *et al* [10]. The solutions for $k = 200\ 000$ to $k = 195\ 000$ are employed for this purpose. More accurate results can be obtained by going to higher k values.

The nature of a small-parameter λ -expansion of the energy function has been a subject of extensive investigation. Bender and Wu [11] concluded on the basis of a

Table 3. Improved bounds for the first three levels ε_{α} , ε_1 , ε_2 of the anharmonic potential $V = x^2 + \lambda x^4$ The first numbers in the energy columns are upper bounds, the second numbers are 'exact' results from [10] and the third numbers are lower bounds. The results for $\lambda = 0$ 1, 1, 10 and 100 are displayed Values of k around 200 000 have been used

	ε	ε,	ε2
$\lambda = 0.1$	1 065 285 509 63	3 306 872 013 99	5 747 959 27
	1 065 285 509 54	3 306 872 01	5 747 959 2
	1 065 285 40	3 306 871 4	5 747 957
$\lambda = 1$	1 392 351 643	4 648 812 714	8 655 049 99
	1 392 351 641	4 648 812 70	8 655 049 9
	1 392 351 0	4 648 810	8 655 041
$\lambda = 10$	2 449 174 078	8 599 003 49	16.635 921 6
	2 449 174 072	8 599 003 4	16 635 921
	2 449 173	8 598 99	16 635 899
$\lambda = 100$	4 999 417 56	17 830 192 8	34 873 984 5
	4 999 417 545	17 830 192	34 873 984
	4 994 13	17 830 172	34 873 93

direct calculation of the perturbation series that it does not converge Further studies were reported by Simon [12]. A good survey of the relevant contributions is provided by Biswas *et al* [10]. Hioe and co-workers [13] have also provided arguments to support the fact that the Taylor expansion has a vanishing radius of convergence.

Within our approach this last fact can be very strongly advocated on the basis of an elementary consideration.

To see this, observe that the conditions $a_{k+2} = 0$ and $2\sqrt{g} \gamma = \lambda$ determine energy as a function of γ . The parameter γ is determined by (4.5). Clearly, γ has a power series expansion in λ within a certain radius of convergence λ_c that depends on k, i.e. on the auxiliary coupling g. As k increases λ_c decreases and so does g. In the same process the auxiliary potential U_2 approaches the anharmonic potential V. Thus, as k increases $U_2 \rightarrow V$ and $\lambda_c \rightarrow 0$. Since $\varepsilon = \varepsilon(\gamma)$, the radius of convergence of the energy expansion is obviously bounded by λ_c .

It is interesting to note that the addition of a suitably tuned sextic term immediately allows one to write down a convergent expansion. For example, for

$$k=0$$
 $\varepsilon_0 = \gamma = 1 + \frac{3}{4}\lambda + \dots$ for small λ

In fact the first-order term in λ is the same as that for the ground state of $V = x^2 + \lambda x^4$. This is not surprising for g is $O(\lambda^2)$.

5. The double-well potential $V = -ax^2 + x^4$

The quantity of great interest here is the splitting Δ between the ground and first excited state energies that controls the tunnelling rate from one well to the other It is generally believed to have an exponential character for deep wells [14]. We shall find that this indeed is the case for the present problem.

Adding the auxiliary potential as before and using quartic scales, we have to solve the equation

$$\psi'' + (\varepsilon + ax^2 - x^4 - gx^6)\psi = 0. \tag{5.1}$$

Polynomial solutions of degree k obtain provided

$$2\sqrt{g} \gamma = 1 \tag{5.2}$$

and

$$\gamma^{3} + a\gamma = \frac{(2k+3)}{2}$$
(5.3)

As usual the condition $a_{k+2} = 0$ determines the energy eigenvalues.

We have two distinct ways for computing Δ .

First we can exploit as before the nominal concavity of the ε -g curve and obtain improved bounds. For large k, i.e. small g, these qualify as excellent estimates of energy levels so that Δ is easily obtained. These results are in excellent accord with numerically computed Δ and those calculated by Keung *et al* [15] using supersymmetric quantum mechanics. Although the bounds obtained for deep wells ($a \ge 10$) are not as close to the energy eigenvalues as they were for corresponding k-values in the examples of the previous sections, the splitting Δ so computed is essentially exact. This somewhat surprising claim is quite easy to understand. For large a, the well is deep and wide. Both the ground and first excited state functions are approximately peaked over the minima of the well. As a increases these minima move further and further out, away from the origin. Thus, in spite of the smallness of the coupling g, the residual sextic term is able to contribute a bit more than it could in the previous examples. Hence, the bounds are marginally less tight than for the single-well potentials Further, as a increases Δ becomes smaller and smaller and hence one would need to know the levels more and more precisely. However, this is not quite the case. As a increases the two levels of interest approach near degeneracy. The corresponding probability distributions become almost indistinguishable from each other wherever they are non-negligible. Hence, the residual sextic term contributes about the same to the two levels. Thus, the wells with large a but very small g correspond to effectively the same Δ as the well with g = 0. Having reduced g to the level of $\sim 10^{-5}$ we are therefore able to determine the splittings extremely accurately using the linear extrapolation mechanism.

The claim just made can be confirmed entirely within our own framework without recourse to any other means This leads us to our second independent estimate of Δ . For this we observe that the energy levels of the auxiliary double-well potential $U_3 = -ax^2 + x^4 + gx^6$ with $g < 5 \times 10^{-5}$ and $a \sim 10$ are amenable to an excellent parabolic fit $\varepsilon = A + Bg + Cg^2$ This is true for both levels of interest. The coefficient A determines ε_0 and ε_1 for the unperturbed quartic double well of interest to us here. In table 4 we collect the results for a = 8, 9, 10 based on this approach. The energies recorded are in complete accord with a fifth-order Runge-Kutta computation in as far as it goes. The results for shallow wells are also in complete accord with Runge-Kutta computations These are not listed in table 4.

Table 4. Estimated ground and first excited state energies ε_0 and ε_1 for the double-well potential $V = -\alpha r^2 + r^4$ based on a parabolic fit for the corresponding levels of the potential $U_3 = -\alpha r^2 + r^4 + g r^6$ for $g \le 5 \times 10^{-5}$ The quantity Δ is the splitting ($\Delta = \varepsilon_1 - \varepsilon_0$) based on these results while Δ_p is the prediction of a fifth order Runge-Kutta computation

4	ε ₀	ε	$\Delta = \varepsilon_1 - \varepsilon_0$	Δ _R
8	-12 136 330 7204	-12 134 814 3452	151638×10^{-3}	1.516×10^{-3}
9	-16 126 186 4549	-16 125 958 5468	$2\ 279\ 08 \times 10^{-4}$	2.28×10^{-4}
10	-20 633 576 7028	-20 633 546 8842	$2.981.86 \times 10^{-5}$	2.98×10^{-5}

Finally, we find that the splittings for $a \ge 8$ are predicted very satisfactorily by the simple empirical formula

$$\Delta = Aa^{3/2} \exp(-Ba^{3/2}) \tag{5.4}$$

with A = 3.063 4012 and B = 0.474 1456.

We have used our results for a = 9 and a = 10 to compute A and B. We then predict $\Delta = 3.434 \times 10^{-6}$ for a = 11 and $\Delta = 3.51 \times 10^{-7}$ for a = 12, in complete accord with known results [15]. Our result for a = 8 is also reproduced. Surprisingly, even for shallower wells (a = 6, 7), (5.4) is fairly accurate. We note that a variational calculation using two peak Gaussian functions also suggests an exponential form for Δ that is less accurate than (5.4).

5. Concluding remarks

For the set of problems discussed in this paper we have shown that the task of implementing the quantization recipe can be replaced by a set of transparent conditions

Energy spectrum of the potential
$$V = ax^2 + x^4$$
 2739

without having to depart from the real problem in any significant way. As a result one is able to determine the energy spectra to as much accuracy as one desires The procedure is clearly applicable to similar problems in higher dimensions.

Having estimated the energies so accurately, we find it pertinent to address the following question. The type of problems in hand do not seem to possess neat closed-form energy expressions. Given this, can one at least find a closed-form representation that is realistic? For the pure quartic potential $V = x^4$, at least, such an expression is indeed empirically constructible. It is

$$t_n = (2n+1)(a+bn+cn^2)^{1/6} + \left(\frac{n+1}{2}\right)^{4/3} \qquad n = 0, 1, 2, \dots$$

Here a = 0.085328, b = 0.0642928 and c = 0.5109453 This formula reproduces the entire quartic spectrum to within 0.16%.

We have also applied our method to the potential $V = x^2 + \lambda x^6$ Adding the auxiliary potential $ax^8 + bx^{10}$ and suitably quantizing the auxiliary couplings a and b one finds a four-term recursion relation that admits one polynomial solution per k—the degree of the polynomial. It is indeed gratifying that the auxiliary couplings a and b turn out to be extremely small and positive Thus, by going up to k = 14 and applying the perturbative correction as explained in section 3 one is already able to bind the first six levels to about 1% of the numerical values for any λ whatsoever, including the pure sextic case ($\lambda \to \infty$).

The conceptual soundness of our approach is obvious. Its efficiency in practice deserves to be mentioned. This can be gauged from the fact that any low-lying quartic level can be estimated to an accuracy of about one part in 10⁶ by investing a computer time (using an HP 9000 and BASIC language programming) of the order of 1 minute.

Next, we invite the reader to an open question in relation to this work. We have seen that as k increases the energy levels of the sequence of auxihary potentials tend to those of the problem in hand. It is then indeed tempting to ask if the limit $k \rightarrow \infty$, i.e. $g \rightarrow 0$, can be implemented If this could be feasible then the power series solutions v(x) for the problem of interest could be viewed as the $k \rightarrow \infty$ limit of a sequence of polynomials of degree k. The difficulty is that one has to impose two conditions $a_{k+2} = 0$ and $a_{k+4} = 0$. How could these be properly implemented simultaneously in the $k \rightarrow \infty$ limit is not clear to us.

In view of the added importance of QES problems, some deeper questions deserve to be noted. So far one knows that QES problems arise due to either an underlying dynamical SL(2, R) symmetry [2] or because the Hamiltonian or the associated Hill determinant can be factorized [3, 7]. It would be interesting to find out if there could be other reasons for their origin, such as, for example, dynamical symmetries other than SL(2, R). The problem of the potential $V = x^2 + gx^6 + ax^8 + bx^{10}$, discussed earlier on in this section, is a case in point. It is easily verified that for tuned values of a, b that lead to polynomial solutions, the associated Hamiltonian has no connection with the SL(2, R) group. Further, one would like to know if a symmetry connection is at all necessary, in the first place, for polynomial solutions to materialize. Specifically, we have in mind the example of an asymmetric one dimensional oscillator (V = $\frac{1}{2}k_1x^2$, x > 0 and $V = \frac{1}{2}k_2x^2$, $x \le 0$). It is an exactly solvable problem whose solutions are Weber functions (see [14]). If $k_1/k_2 = [(2n_2+1)/(2n_1+1)]^2$ there appear an infinite but incomplete set of polynomial solutions. As far as one can tell, there appears to be no symmetry connection here at all. The problem does not belong to the Turbiner class [2] and the Hamiltonian is not factorizable à la Leach [3].

2740 S C Chhajlany et al

Finally, a very pertinent question to ask is about the criteria that the manifestly normalizable solutions of a problem obtained by tuning parameters are indeed physical. This question arises because such tuning of parameters can also permit formally divergent solutions of certain multiple-term recursion relations to collapse into polynomials and thus become normalizable at tuned values of coupling constants. Upon relaxing the tuning condition they follow a divergent path in the parameter space of such auxiliary couplings. An explicit example of such a circumstance has recently been pointed out by Chhajlany and Malnev [16]. Of course, we must note that such an unhappy circumstance does not obtain with our solutions here. They originate in an underlying symmetry, continue to the verifiable correct limits and the energy predictions based on them for arbitrary coupling constant values other than the tuned values are demonstrably correct.

The accomplishments of this work can be summed up as follows, des problems have been extensively studied in the literature and have generally been considered to be of limited utility. We have demonstrated that this is indeed not so. They provide meaningful estimates of energy eigenvalues for other problems that are not oes. The procedure is conceptually sound, avoids troublesome questions such as those pertaining to normalizability and the nature of small-parameter expansions. The method works for any level and any anharmonicity in the cases considered. At the same time, approximate polynomial wavefunctions related to underlying symmetry groups obtain as viable substitutes for the exact wavefunctions that are not available. Given the computational facilities, very accurate numerical results can be obtained. Accuracies of about one part in 10¹⁰ have been demonstrated and greater accuracies are clearly achievable. On the practical side the method works on essentially the same lines as the Hill determinant approach so that the practical methodology of the latter comes in quite handy. For useful results both methods require roots of very large-size determinants. However, in both cases the determinants have simple structures (tridiagonal form in the principal cases discussed) that substantially facilitate the evaluation of roots. We find that for large-size determinants the Hill determinant approach produces superior numerical results. The difference arises due to the presence of non-zero auxiliary contributions in our case. On the other hand the Hill approach requires a separate proof of normalizability and the wavefunctions formally remain power series functions which can never be exact as far as any practical calculation goes.

On the computational side there are a host of other methods which are decisively more efficient whenever they apply. We briefly review a selected few. Following a chronological sequence we begin with the elegant approach of intermediate Hamiltonians due to Bazley and Fox [17]. It provides excellent lower bounds extremely efficiently for low-lying states of anharmonic and other potentials. The conceptual basis of this method is very transparent and very small-size (-5×5) determinants are needed. Results obtained for weak and medium anharmonicities are very impressive indeed. The Hill determinant approach [9, 10] has already been noted. Next comes the two-step approach of Cheng-Shiung Hsue and Chern [18] using coherent states, which is also able to extract very accurate estimates using small-size determinants (-20×20) . They have also discussed all the three main problems we have considered. There is no criterion here to decide whether a given estimate is ar upper or a lower bound. Another powerful approach is the method of moments due to Bessis and Handy [19]. Again good results (lower bounds) obtain with ease. The method needs special adaptations to treat excited states and the Killingbeck problem has also been examined using this approach [20]. From a numerical point of view and to the best of our knowledge the most striking accuracies using small-size determinants (7×7) are obtainable through the rational function approach of Fernandez *et al* [21], which applies to a wide variety of potentials, although double-well potentials have not been explicitly mentioned by the authors. The method successively obtains tighter and tighter upper and lower bounds as the determinant size increases in steps of one. As an example, using 7×7 determinants the first four quartic levels are estimated to one part in 10^{12} . The authors have been unable to provide a theoretical reason for the emergence of successive upper and lower bounds.

A general observation concerning the methods of the previous paragraph is in order. Unlike our and the Hill determinant-based approaches the above methods involve general $N \times N$ determinants. Thus, whereas their computational superiority for the case of low-lying states is beyond doubt, the same need not be true for the case of highly excited states such as the 100th level Unfortunately, these authors have not shown such cases and we are unable to add anything more in relation to this question.

The above has been a very limited review and a number of other useful approaches such as Pade-Borel summability techniques for the weak coupling case and 1/N expansion-based methods, etc, have been left unattended. However, their accomplishments can be traced through [1, 10, 13].

Finally, we note that we are in the process of applying the present method, which may be termed as the method of auxiliary Hamiltonians, to the Coulomb-diamagnetic and the Coulomb-plus linear potential problems. Preliminary results in the Coulombdiamagnetic case indicate that an excellent description of the Coulombic and quasi-Landau regimes obtains. The details of these and some other applications will be discussed elsewhere.

References

- [1] Chhajlany S C and Malnev V N 1990 Phys Rev. A 42 3111
- [2] Turbiner A V 1988 Commun Math Phys 118 467
- [3] Leach P G L 1985 Physica 17D 331
- [4] Leach P G L, Flessas G P and Gorringe V M 1989 J. Math Phys 30 406
- [5] Dutta A K and Willey R S 1988 J Math Phys 29 892
- [6] Calogero F 1979 Lett. Nuovo Cimento 25 323
- [7] Singh V, Biswas S N and Dutta K 1978 Phys. Rev D 18 1901
- [8] Saxena R P and Varma V S 1982 J Phys. A: Math. Gen 15 L221 Varma V S 1981 J Phys. A. Math. Gen. 14 L481
- [9] Banerjee K, Bhatnagar S P, Choudhary V and Kanwal S S 1978 Proc. R Soc London A 360 575
- [10] Biswas S N, Dutta K, Srivastava P K and Varma V S 1973 J. Math Phys. Rev 9 1190
- [11] Bender C and Wu T T 1969 Phys Rev 184 1231
- [12] Simon B 1970 Ann. Phys., NY 58 76
- [13] Hioe F T, Macmillen D and Montroll E W 1978 Phys Rep. 43C 305
- [14] Landau L D and Lifshitz E 1977 Quantum Mechanics (New York Pergamon) Merzbacher E 1970 Quantum Mechanics (New York Wiley)
- [15] Keung W Y, Kovacs E and Sukhatme V P 1988 Phys Rev Lett. 60 41
- [16] Chhajlany S C and Malnev V N 1991 Phys Rev. A 43 581
- [17] Bazley N and Fox D 1961 Phys Rev. 124 483
- [18] Chen-Shiung Hsue and Chern J L 1984 Phys Rev D 29 643
- [10] Handy C and Bessis D 1985 Phys. Rev Lett 55 931
- [20] Bessis D, Vrscay E R and Handy C R 1987 J. Phys A: Math Gen. 20 419
- [21] Fernandez F M, Ma Q and Tipping R H 1989 Phys Rev A 39 1605