

## The harmonic oscillator with $\lambda x^M$ perturbation

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1980 J. Phys. A: Math. Gen. 13 49

(<http://iopscience.iop.org/0305-4470/13/1/007>)

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 30/05/2010 at 20:04

Please note that [terms and conditions apply](#).

## The harmonic oscillator with $\lambda x^M$ perturbation

J Killingbeck

Physics Department, University of Hull, Hull HU6 7RX, UK

Received 23 February 1976, in final form 30 May 1979

**Abstract.** Perturbation theory is applied to improve the accuracy of a numerical integration method for the Schrödinger equation. The resulting method is applied to the special case of the perturbed oscillator problem in order to obtain energy perturbation coefficients for the case in which the  $x^2$  term is taken as the perturbation.

### 1. Introduction

The energy levels of the perturbed harmonic oscillator Hamiltonian

$$H(\mu, \lambda) = -D^2 + \mu x^2 + \lambda x^M \quad (1)$$

have been most studied for the case  $\mu = 1, M = 4$ . This particular case has been treated by the WKB method (Bender and Wu 1968), by Padé approximant methods (Loeffel *et al* 1969, Simon 1970), by the intermediate Hamiltonian method (Bazley and Fox 1961), by Heisenberg matrix mechanics (Chasman 1961), and by variational methods (Schwartz 1965, Reid 1970, Truhlar 1971). The Hamiltonian (1) with  $\mu = 1, M = 6$  or 8 has been treated by the WKB method (Banks and Bender 1972), by Borel–Padé summation techniques (Graffi *et al* 1971), by a recurrence relation method (Biswas *et al* 1973), and by a simple power series method (Secrest *et al* 1962). In fact, the last method gives the best results for  $M = 6$  or 8 without the lengthy calculations which are needed for the matrix-variational approach or the Padé approximant approach. That the Rayleigh–Schrödinger perturbation series in powers of  $\lambda$  for any eigenvalue  $E(\mu, \lambda)$  of the Hamiltonian (1) will diverge for  $M > 2$  was noted by Frank (1967) on general grounds. Although a Padé approximant summation of the  $\lambda$  perturbation series succeeds for  $M = 4$  and  $M = 6$ , it does not do so for  $M = 8$ , since the even- and odd-order Padé approximant sequences for the energy series do not have a common limit (Graffi and Grecchi 1978). A modified Borel–Padé method will work for  $M = 8$  (Graffi *et al* 1971), but is not a very practical method for calculating  $E(\mu, \lambda)$ , since even a  $\lambda$  value of  $10^{-3}$  (with  $\mu = 1$ ) counts as ‘large’ for that method. Most of the methods referred to above need double-precision computation because they involve calculating many matrix elements or perturbation coefficients; Biswas *et al* (1973) noted that their method involved a prohibitive amount of computer time for  $M = 8$ , so that some of their quoted eigenvalues had converged to only two decimal places.

In the present work we exploit the fact that the Hamiltonian (1) can be treated very effectively if the  $\mu x^2$  term is treated as the perturbation, with  $\lambda$  held fixed at the value  $\lambda = 1$ . Simon (1970) actually used this point of view in his formal considerations, but then treated  $\lambda$  as the perturbation parameter in the numerical portion of his paper,

where he studied high-order Padé approximants based on the  $\lambda$  series. If we set  $\lambda = 1$ , and apply the usual theorems about regular perturbations, as summarised by Simon (1970), we conclude that the perturbation series in  $\mu$  for the eigenvalue  $E(\mu, 1)$  will be a convergent one (for  $\mu$  sufficiently small). For the case  $M = 4$  Simon (1970) gives a scaling argument, which we can easily modify to apply to other  $M$  values. It leads to the relation

$$E(1, \lambda) = \lambda^{1/n} E(\lambda^{-2/n}, 1) \quad (2)$$

where the integer  $n$  is given by  $n = \frac{1}{2}M + 1$ . The result (2) shows that for large  $\lambda$  the perturbation series for  $E(\mu, \lambda)$  will take the form

$$E(\mu, \lambda) = \lambda^{1/n} (E_0 + E_1 \mu \lambda^{-2/n} + E_2 \mu^2 \lambda^{-4/n} + \dots) \quad (3)$$

where the coefficients  $E_n$  (which we expect to decrease rapidly with  $n$ ) are the perturbation coefficients for the expansion of  $E(\mu, 1)$  in powers of  $\mu$ . In §§ 2 and 3 we discuss various methods of finding  $E(\mu, 1)$  and the  $E_n$ , in § 4 we discuss the calculation of various expectation values, and in § 5 we present the results for the two lowest even-parity eigenstates for  $M = 4, 6$  and  $8$ . The series (3) works well in the strong perturbation ( $\lambda > 1$ ) region where methods based on the  $\lambda$  series are of little use. It is obviously more economical to give the  $E_n$  coefficients than to give a lengthy table of  $E(\mu, 1)$  values for selected  $\mu$  values. We should point out that from the series (3) we can obtain by partial differentiation the series for  $\langle x^2 \rangle = \partial E / \partial \mu$  and  $\langle x^M \rangle = \partial E / \partial \lambda$ .

## 2. Variational and hypervirial approaches

Although the perturbation series in  $\lambda$  for  $E(1, \lambda)$  diverges rapidly, it does have coefficients which can in principle be calculated exactly, since the unperturbed wavefunction (at  $\lambda = 0$ ) is a harmonic oscillator function. Bender and Wu (1968) gave the first 75 coefficients for the case  $M = 4$ . On the other hand, the series in  $\mu$  for  $E(\mu, 1)$  is a quickly converging one, but the coefficients must be calculated numerically, since the unperturbed wavefunction (at  $\mu = 0$ ) is an unknown function. For  $M = 4$ , it is possible to find an exact ground-state eigenfunction for a harmonic oscillator perturbed by a sum of  $x^4$  and  $x^6$  terms, and use that as an exact unperturbed function (Killingbeck 1978). Here we wish to find a method which works equally well for  $M = 6$  and  $8$ .

The use of the  $\mu x^2$  term as the perturbation has been tried before in numerical work, by Chan *et al* (1964) for the case  $M = 4$ . Although we proceed by a different route, we can comment on the relevance of the method of this paper to their work. They proceed by using an oscillator-type basis and a matrix diagonalisation method to obtain several energy levels and wavefunctions for the case  $\mu = 0$ . They then evaluate the matrix elements of  $\mu x^2$  between these functions and use them in a new matrix calculation to get the levels for  $\mu > 0$ . They also work out the second-order energy shift due to the  $\mu x^2$  perturbation, apparently by using their matrix elements in a truncated sum-over-states calculation. In terms of the ideas of the present paper, their approach could be developed more compactly as follows. By finding  $E_0$  and  $\langle \psi_0 | x^2 | \psi_0 \rangle$  for the ground state only at  $\mu = 0$ , we can find the higher  $\langle \psi_0 | x^N | \psi_0 \rangle$  easily from hypervirial relations; such relations have been known for a long time, but have been used recently in this way by, for example, Tipping (1976) and Killingbeck (1979). The basis states  $x^N \psi_0$  can then be used to set up the Hamiltonian matrix, or to set up a Hylleraas variational principle for

the second-order energy, if we use the identity (Killingbeck 1979)

$$\langle \psi | x^M (H - \epsilon) x^N | \psi \rangle = MN \langle \psi | x^{M+N-2} | \psi \rangle, \quad (4)$$

which holds for any eigenfunction  $\psi$ , with energy  $\epsilon$ , associated with the Hamiltonian  $H$ .

Richardson and Blankenbecler (1979) have developed the use of hypervirial relations to permit the numerical calculation of energies and  $\langle x^N \rangle$  values for Hamiltonians such as (1). The gist of their method is that the asymptotic form of the wavefunction as  $|x| \rightarrow \infty$  is known if  $M$  is given, and that it is the large  $x$  region which dominates in the calculation of  $\langle x^N \rangle$  if  $N$  is large. By starting from a large  $N$  value and working back to low  $N$  values using the hypervirial relations, it is possible to obtain self-consistent estimates for the energy  $E$  and the  $\langle x^N \rangle$ . It seems that a starting value  $N > 1024$  is needed to get a stable result for the first five decimal places in  $E$ ; numerical results are only given for  $M = 4$  by Richardson and Blankenbecler (1979).

Hioe *et al* (1975, 1976) treated the perturbed oscillator problem for  $M = 4, 6$  and  $8$  by using the Bargmann representation. For our Hamiltonian (1) their procedure would involve changing to the Hamiltonian

$$H = \left( 1 + z \frac{d}{dz} \right) + \lambda \left[ \frac{1}{2} \left( z + \frac{d}{dz} \right) \right]^M \quad (5)$$

(for the case  $\mu = 1$ ), and noting that the functions  $z^N$  are the eigenfunctions at  $\lambda = 0$ . Using the  $z^N$  as basis functions for the case  $\lambda > 0$  leads to determinantal equations which must be truncated at some  $N$  value.  $N > 20$  seems to be needed to find the energy to five decimal places at  $\lambda = 1$ . For large  $\lambda$  values, Hioe *et al* (1976) give a relation equivalent to (2) of this paper, and convert their problem to an equivalent weak perturbation problem. They were the first authors to give some perturbation coefficients  $E_n$  for the large  $\lambda$  case, and for  $M > 4$ , although their calculations are not accurate enough to go beyond  $E_2$ ; we have converted their results into our units and have displayed them for comparison in tables 1 and 2. (Their quoted  $E_0$  value for  $M = 4$  is in error, probably because of a misprint.)

Banerjee and Bhatnagar (1978) treated the  $M = 4$  case by using a trial function equal to the product of a power series and a scaled ground-state oscillator wavefunction. Their method involves large determinants; we note that the method of Secrest *et al* (1962) would probably work more efficiently if it also used such trial functions, rather than using a power series on its own.

**Table 1.** Ground-state perturbation coefficients.

$M$	4	6	8
$E_0$	1.060 362 090 (1.060 362 090)†	1.144 802 454 (1.144 808)	1.225 820 114 (1.225 82)
$E_1$	0.362 022 65 (0.362 03)	0.307 920 30 (0.307 74)	0.277 118 93 (0.2768)
$E_2$	-0.034 5096 (-0.035)	-0.018 5417 (-0.0175)	-0.012 6323 (-0.0118)
$E_3$	0.005 195	0.001 560	0.000 751
$E_4$	-0.000 90	-0.000 12	-0.000 04

† Bracketed values from Hioe *et al* (1976).

**Table 2.** Excited-state perturbation coefficients.

$M$	4	6	8
$E_0$	7.455 697 938 (7.455 697 94)†	9.073 084 560 (9.073 09)	10.244 946 977 (10.2449)
$E_1$	1.244 714 12 (1.244 73)	0.904 435 59 (0.904 49)	0.752 344 97 (0.7526)
$E_2$	-0.046 6015 (0.050)	-0.010 2493 (-0.0108)	-0.003 0708 (-0.0036)
$E_3$	0.000 959	-0.000 749	-0.000 520
$E_4$	0.000 36	0.000 11	0.000 02

† Bracketed values from Hioe *et al* (1976).

### 3. A direct calculation of the $E_n$

The most simple approach to finding the first few  $E_n$  is to calculate  $E(\mu, 1)$  very accurately for several small  $\mu$  values and then extract the  $E_n$  by numerical differencing. This approach can be used equally well for any eigenvalue, and is the one adopted here. The basic problem then becomes that of calculating the energy. A study of the works cited in the Introduction makes it quite clear that for a simple Hamiltonian such as (1) the use of some kind of direct numerical integration procedure is both more easy and more accurate than the use of large matrices. The method which we use will actually work just as easily for perturbations such as  $\lambda x^2(1 + gx^2)^{-1}$ ; in a matrix approach such potentials require numerical integration to find the matrix elements, as well as the diagonalisation of large matrices (Mitra 1978).

The method is very simple but effective, and is outlined here for a Schrödinger equation (with a local potential) in the form

$$D^2\psi(x) = [V(x) - E]\psi(x) = \phi(x)\psi(x). \quad (6)$$

The quantity which we study is  $\delta^2\psi$ , defined by

$$\delta^2\psi = h^{-2}[\psi(x+h) + \psi(x-h) - 2\psi(x)]. \quad (7)$$

Here  $h$  is the small strip width to be used in the numerical integration. Use of the Taylor expansion and of equation (6) quickly gives us

$$\delta^2\psi = \phi\psi + \frac{1}{12}h^2D^4\psi + \dots \quad (8)$$

The equation  $\delta^2\psi = \phi\psi$  can be treated using step-by-step integration, since  $\delta^2$  of equation (7) has replaced the differential operator  $D^2$ . This method works quite well (Killingbeck 1977b), but can be improved by taking into account the  $h^2$  term in (8) also. If we think of  $\frac{1}{12}h^2D^4$  as a perturbation operator, giving the difference between the true Hamiltonian and our finite difference version of it, then according to first-order perturbation theory the energy shift  $E_1$  caused by this perturbation is given by  $E_1 = \langle \psi | \frac{1}{12}h^2D^4 | \psi \rangle$ . Here  $\psi$  is the exact eigenfunction of the correct Hamiltonian. However, we know that equation (6) is obeyed by that function, and can quickly show that  $E_1 = \frac{1}{12} \langle \psi | \phi^2 | \psi \rangle$ , provided that  $V$  is finite at the origin and that  $\psi$  goes to zero suitably at infinity. This result means that we can correctly allow for the energy shift

caused by the  $D^4$  term if we replace it by the more simple term  $\phi^2$ , so that our finite-difference equation takes the form

$$\delta^2\psi = \phi\psi + \frac{1}{12}h^2\phi^2\psi. \quad (9)$$

Strictly speaking, the derivation above is supposing that  $\phi$  equals  $(V - E)$ , where  $E$  is the exact eigenvalue of the Schrödinger equation. What we do in practice is to use a trial  $E$  value in (9) and integrate outwards from the origin until we reach a critical region where  $\psi$  either changes sign or begins to diverge upwards. Proceeding a little further, to some distance  $x_0$ , we note the  $\psi$  value. Repeating for a slightly different trial energy  $E^1$  we obtain two numbers,  $\psi(x_0, E)$  and  $\psi(x_0, E^1)$ . Linear interpolation using these  $\psi$  values gives us a good estimate of the energy value which would have produced a zero  $\psi$  value at  $x = x_0$ . In practice, this interpolation procedure is surprisingly accurate, reducing the error by factors of up to  $10^3$  at each step. It is quite easy to devise a program (for example, for a TI 58 calculator) which does the outward integration simultaneously for two close  $E$  values and yields the interpolated  $E$  value as output. Only three or four runs are needed to produce an  $E$  value accurate to  $10^{-9}$  or less; this  $E$  refers to the specific  $h$  value used in (9) and should be labelled  $E(h)$ . What we need is the  $E$  value for the limit  $h \rightarrow 0$ . The perturbation theoretic derivation of (9) implies that there is a series expansion of the form

$$E(h) = E(0) + \epsilon_4 h^4 + \epsilon_6 h^6 + \dots \quad (10)$$

since the  $\phi^2$  term in (9) was designed to suppress the  $h^2$  error term which appeared in the earlier method used by Killingbeck (1977b). The validity of (10) has also been confirmed numerically by calculations on various test potentials. To find  $E(0)$ , then, we find  $E(h)$  for a few different  $h$  values and extrapolate. For the problems of this paper use of two  $h$  values (e.g. 0.02 and 0.04) was found to be adequate to give a final  $E(0)$  value accurate to nine decimal places (for the TI 58 calculator). The few results given to that accuracy by earlier workers (e.g. Reid 1970, Secret *et al* 1962) were reproduced correctly by our method. Finding  $E(\mu, 1)$  values to this accuracy for a selection of small  $\mu$  values (e.g. 0,  $\pm 0.05$ ,  $\pm 0.1$ ) makes it possible to extract stable estimates of the low-order perturbation coefficients, and these are shown in table 1. (To treat the first excited state, the wavefunction  $\psi$  is allowed to have one node before the critical region is reached, but otherwise the procedure is the same as that for the ground state.)

#### 4. Expectation value calculations

It is traditionally regarded as much harder to find the accurate wavefunction than to find the eigenvalue  $E$ . However, the wavefunction is most often *used* to calculate expectation values, and it is possible to find these quite accurately by the method of § 3. There are two main ways in which to find expectation values:

(a) *Direct integration.* The integrals of  $\psi^2 f(x)$  and  $\psi^2$  are constructed as equation (9) is integrated outwards, and the expectation value  $\langle f(x) \rangle$  found by taking the ratio of the integrals.  $\psi(0)$  can be arbitrarily set equal to 1 to start off the integrations. For finite  $h$ , of course, the result is not the required  $\langle f(x) \rangle$ , but the relation

$$\langle f(x) \rangle_h = \langle f(x) \rangle_0 + f_2 h^2 + f_4 h^4 + \dots \quad (11)$$

holds. Accordingly, using two  $h$  values to find the energy  $E$  permits us simultaneously to work out  $\langle f(x) \rangle$  by evaluating the appropriate integrals for any function  $f(x)$ . There is

one subtlety involved in the accurate evaluation of  $\langle f(x) \rangle_h$ . We want to find  $\langle f(x) \rangle_h$  for the correct  $E(h)$  value, whereas in practice two trial values are used for  $E$ . When  $E$  is accurately known, so that the two trial  $E$  values differ by, say,  $10^{-9}$ , the calculated  $\langle f(x) \rangle$  differ by a similarly small amount, provided that we take their values at  $x = X_0$ . Here  $X_0$  is the  $x$  value at which  $\psi$  has the node, and is less than the  $x_0$  used in the energy interpolation. The divergent region of  $\psi$  (with  $x > X_0$ ) gives increasing contributions which 'spoil' the integrals; the true wavefunction would be almost zero in that region. The numerical results indicate that this procedure yields values of  $\langle x^n \rangle$  for the eigenfunctions of the Hamiltonian (1) which are accurate to much better than 1 part in  $10^6$ . By modifying an argument given by Froman (1978), we can express the value of the squared wavefunction at  $x = 0$  in terms of an expectation value of the modulus of the derivative of the potential

$$\langle |DV| \rangle = [E - V(0)]\psi^2(0). \quad (12)$$

(b) *The eigenvalue approach.* This approach uses the Hellmann–Feynman theorem (equivalent to first-order perturbation theory) and involves accurate computation of the energy eigenvalue for the Hamiltonian (1) with the small perturbing term  $\pm\alpha f(x)$  included.  $\alpha$  is small (typically  $10^{-3}$ ) and the expectation value  $\langle f(x) \rangle$  then follows by differencing:

$$E(+\alpha) - E(-\alpha) = 2\alpha \langle f(x) \rangle. \quad (13)$$

This approach has the beautiful feature that it reduces the calculation of expectation values to the calculation of energy values, which we can do accurately, without the need for producing the detailed wavefunction as an intermediate product. It would work for any computational method which gives accurate energy values, but is particularly useful here. If the approach is used in a matrix calculation it yields nothing new; the use of (13) then yields exactly what would be found by directly calculating  $\langle f(x) \rangle$  using the approximate eigenvector associated with the approximate eigenvalue. The present calculation uses  $\mu x^2$  as a perturbation in the Hamiltonian (1) (with  $\lambda = 1$ ); the first-order energy coefficient is thus directly equal to the expectation value  $\langle x^2 \rangle$  for the unperturbed ( $\mu = 0$ ) wavefunction.

To ensure that the direct integration method of (a) is carried out using a reliable wavefunction we introduced the function  $F(x)$ , defined by the relation

$$\psi(x+h) = [1 + h^2 F(x)]\psi(x). \quad (14)$$

Inserting this definition into (9) leads to the recurrence relation

$$F(x) = F(x-h)[1 + h^2 F(x-h)]^{-1} + \phi + \frac{1}{12}h^2\phi^2 \quad (15)$$

with  $\phi = V - E$ . Equation (15) allows  $F$  to be found very accurately at each  $x$ , and  $\psi$  can be constructed from it using (14). This approach gives less cumulative rounding error than the method which uses  $\psi(x \pm h)$  and  $\psi(x)$  directly in the recurrence relation resulting when (7) is substituted in (9). This has been confirmed in various test calculations but can be seen in principle by noting that the  $x$ -dependent term  $h^2 F$  is typically small compared with unity and so is 'masked' by the unity term if the function  $1 + h^2 F$  is calculated directly at each step. The obvious internal check on the methods of this section is to compare the values of  $E_1 = \langle x^2 \rangle$  as obtained by the two methods. The results at  $\mu = 0$  for  $M = 4, 6$  and  $8$  showed that the  $\langle x^2 \rangle$  values from the two methods agree to within  $10^{-7}$  for both the states considered. Either of the methods would thus suffice to give  $\langle x^n \rangle$  values to be used in the kind of calculation outlined in § 2.

### 5. Results and discussion

Tables 1 and 2 show the results for the  $E_n$ , for the first two even-parity states, as obtained by numerical differencing from the eigenvalues at  $\mu = 0, \pm 0.05, \pm 0.1, \pm 0.2$ . The error  $(E - S_4)$ , where  $E$  is the true energy and  $S_4$  the sum of the series (3) up to the  $E_4$  term, is somewhat less than the size of the fourth-order term for  $\mu = 1$  and  $\lambda > 1$ , and  $S_4$  gives the energy to sufficient accuracy for most purposes. The resulting eigenvalue estimates for  $M = 6$  or  $8$  are much more accurate than those of Biswas *et al* (1973). In the case  $M = 2$  an analytic solution shows that every eigenvalue of the Hamiltonian varies as  $(\lambda + \mu)^{1/2}$ , so that the perturbation coefficients  $E_n$  alternate in sign. The excited state results show, however, that for  $M = 6$  or  $8$  the signs of *both*  $E_2$  and  $E_3$  are negative, and suggest that for  $M = 5$  the value of  $E_3$  for the first even-parity excited state passes through a zero when considered as a function of  $M$ .

One feature of the methods of §§ 3 and 4 should be particularly stressed. In the numerical treatment of the Schrödinger equation it is always easier to get an accurate energy value than to obtain an accurate eigenfunction. Furthermore, the storage of the wavefunction in numerical form takes up a large amount of storage capacity. In practice, however, the wavefunction is not often used in isolation, but is combined with operators to form expectation values. The work of this paper shows how (for one-particle problems) much of the theory can be directly reduced to involve only eigenvalue calculations, which are the easiest ones to carry out. The method of § 4(a) does allow the extraction of  $\psi$  if desired (for  $x$  values between the origin and the critical region), but most of the traditional calculations of quantum mechanics could be performed without direct knowledge of  $\psi$ .

When comparing the numerical results of this work with those of previous authors it is important to note that the majority of works quote tables of  $E(\lambda)$  for selected  $\lambda$  values and for  $\mu = 1$ . Since the results are usually quoted to less than nine decimal places, the method of § 3 is more accurate (and simpler) in almost all cases; even the few exceptions would be removed if we used double-precision computation (as they do). The series of equation (3) will permit more speedy estimation of  $E(\mu, \lambda)$  at variable values of the parameters, and given this estimated  $E(\mu, \lambda)$  we can refine it using the method of § 3. This refining process is not possible for most of the other methods, except that of Secrest *et al* (1962); our method, incidentally, will provide an  $x_0$  value which will quickly define the basic region ( $x < x_0$ ) to be used in their method. The individual Padé approximants of Simon (1970) for  $M = 4$  are quoted to twelve figures, but when we attempt to derive  $E(1, 1)$  from them as a limit it is only found to four decimal places. The result is  $E(1, 1) = 1.3923$ , whereas  $S_4$  from our perturbation series is 1.392 17, which becomes 1.392 30 if we continue the series as a geometric series. Table 3 compares some  $S_4$

**Table 3.** Specimen  $E(1, \lambda)$  values for  $M = 6$  and  $8$ .

$\lambda$	$E_0(6)$	$E_2(6)$	$E_0(8)$	$E_2(8)$
1	1.435 6246† (1.435 6211)‡	9.966 622 (9.966 6318)	1.490 - 1 (1.491 0177)	10.993 - 4 (10.993 7211)
10	2.205 7232 (2.205 7233)	16.641 21 (16.641 2182)	2.115 - 22 (2.114 5446)	16.707 - 15 (16.711 0217)

† From Biswas *et al* (1973).

‡  $S_4$  value.



values from our series with the results of Biswas *et al* (1973). With so few terms of the series it is difficult to say anything about the radius of convergence. It seems to be about 5 if we look at the ratios of successive coefficients (for the  $M = 4$  ground state), but the comments of Banerjee and Bhatnagar (1978) suggest that we might expect trouble at the  $\mu$  value ( $-3.3$ ) at which there arise four classical turning points in the classical motion. (For  $\mu < 0$  the potential has two wells in it.) In a preliminary investigation of this point we have calculated  $E(\mu, 1)$  in the region around  $\mu = -3.3$ , but cannot find any apparent discontinuity in  $E(\mu, 1)$  or its low-order derivatives.

## References

- Banerjee K and Bhatnagar S P 1978 *Phys. Rev. D* **18** 4767–9  
 Banks T I and Bender C M 1972 *J. Math. Phys.* **13** 1320–4  
 Bazley N and Fox D 1961 *Phys. Rev.* **124** 483–92  
 Bender C and Wu T T 1968 *Phys. Rev. Lett.* **21** 406–9  
 Biswas S N, Datta K, Saxena R P, Srivastava P K and Varma V S 1973 *J. Math. Phys.* **14** 1190–5  
 Chan S I, Stelman D and Thompson L E 1964 *J. Chem. Phys.* **41** 2828–35  
 Chasman R 1961 *J. Math. Phys.* **2** 733–5  
 Frank W M 1967 *J. Math. Phys.* **8** 1121–7  
 Fröman N 1978 *Phys. Rev. A* **17** 493–504  
 Graffi S and Grecchi V 1978 *J. Math. Phys.* **19** 1002–6  
 Graffi S, Grecchi V and Turchetti G 1971 *Nuovo Cim. B* **4** 313–40  
 Hioe F T, MacMillen D and Montroll E W 1975 *J. Math. Phys.* **16** 1945–55  
 ——— 1976 *J. Math. Phys.* **17** 1320–37  
 Killingbeck J 1977a *Rep. Prog. Phys.* **40** 963–1031  
 ——— 1977b *J. Phys. A: Math. Gen.* **10** L99–103  
 ——— 1978 *Chem. Phys. Lett.* **55** 303–4  
 ——— 1979 *Phys. Lett. A* in press  
 Loeffel J J, Martin A, Simon B and Wightman A S 1969 *Phys. Lett.* **30B** 656–8  
 Mitra A K 1978 *J. Math. Phys.* **19** 2018–22  
 Reid C 1970 *J. Molec. Spectrosc.* **36** 183–91  
 Schwartz C 1965 *Ann. Phys., NY* **32** 277–91  
 Secrest D, Cashion K and Hirschfelder J D 1962 *J. Chem. Phys.* **37** 830–5  
 Simon B 1970 *Ann. Phys., NY* **58** 76–136  
 Tipping R H 1976 *J. Molec. Spectrosc.* **59** 8–12  
 Truhlar D G 1971 *J. Molec. Spectrosc.* **38** 415–21