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1989 J. Phys. A: Math. Gen. 22 61

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## Splitting in a double-minimum potential with almost twofold degenerate lower levels

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Received 19 July 1988

**Abstract.** An analytic continuation procedure using Taylor series is utilised to produce very accurate wavefunctions and eigenvalues for a double-minimum potential having almost degenerate eigenvalues. Comparison is made with results obtained by other means.

### 1. Introduction

Double-minimum potentials occur in several areas of physics, and a variety of techniques have been used over the years to investigate their eigenvalues and other properties (Morse and Stueckelberg 1931, Dennison and Uhlenbeck 1932, Wu 1933, Somorjai and Hornig 1962, Chan and Stelman 1963, Ezawa *et al* 1970, Fröman *et al* 1972, Polyakov 1977, Brezin *et al* 1977, Gildener and Patrascioiu 1977, Banerjee and Bhatnagar 1978, Zhirnov and Turev 1980, Pajunen 1980, Balsa *et al* 1983, Bhattacharya 1985). One such potential which has frequently been studied is the following:

$$V(x) = -kx^2 + \lambda x^4 \quad k, \lambda > 0. \quad (1)$$

Its eigenvalue spectrum has the feature that the lower eigenvalues are closely bunched in pairs if the two wells are sufficiently separated. The Hamiltonian for the potential (1) can be written as

$$H(k, \lambda) = p^2 - kx^2 + \lambda x^4 \quad p = -id/dx. \quad (2)$$

As pointed out by Banerjee and Bhatnagar (1978), from the scaling ( $x \rightarrow ax$ ,  $p \rightarrow a^{-1}p$ ) properties of the Hamiltonian  $H(k, \lambda)$  it follows that  $H(k, \lambda)$  and  $a^{-2}H(a^4k, a^6\lambda)$  are unitarily equivalent and therefore have the same eigenvalues. Hence  $E_n(k, \lambda) = k^{1/2}E_n(1, \lambda')$ ,  $\lambda' = k^{-3/2}\lambda$ . Thus one need only consider the eigenvalue problem of the reduced Hamiltonian  $H(1, \lambda) = p^2 - x^2 + \lambda x^4$ .

For accurate calculation of the eigenvalues of close-lying levels in double-minimum potentials, numerical methods have increasingly been used in recent years (Kolos and Wolniewicz 1969, Lin 1974, Tobin and Hinze 1976, Truhlar and Tarara 1976, Wicke and Harris 1976, Johnson 1977, Wolniewicz and Orlikowski 1978, Talman 1980). The most unfavourable conditions for a numerical integration arise when the potential in question has almost degenerate eigenvalues. One such potential was investigated by Wolniewicz and Orlikowski (1978) (wo):

$$V(x) = 200(3x^6 - 6x^2 - 1) \quad (3)$$

with symmetric boundary value conditions

$$y(-2) = y(2) = 0. \quad (4)$$

The lower levels for this potential are almost twofold degenerate (to almost 1 part in  $10^{14}$ ) and consequently this problem is numerically difficult. wo computed the eigenvalues for (3) by the bisection method and also by the Cooley method. Talman (1980) used a modification of the Cooley method to calculate the six lowest levels of the same potential. An inspection of the results of wo and Talman (1980) shows that there are considerable differences in the results of these two studies.

Recently one of the authors (Hodgson 1988a, b) has used an analytic continuation procedure using Taylor series to produce very accurate wavefunctions and eigenvalues for the Schrödinger equation. This method was first proposed by Holubec and Stauffer (1985) for scattering problems. So far this method has only been used for single-well potentials. In the present paper we have applied this method to potential (3) in order to resolve discrepancies in the existing values. To check the accuracy of this method for double-minimum potentials, we have also carried out calculations for certain values of the parameters in potential (1) which were used by Balsa *et al* (1983).

## 2. Procedure

The standard Taylor series approach to the solution of a differential equation (DE) with initial values given at  $z_0$  is to approximate the solution in the neighbourhood of  $z_0$  by a truncated Taylor series. The values of the derivatives at  $z_0$  are determined from successive differentiations of the DE. One then proceeds to construct a new Taylor series about  $z_1 = z_0 + h$  using the derivatives of the first series. This process continues to generate an analytic continuation of the solution of the DE along the path  $\{z_0, z_1, z_2, \dots\}$ . This technique requires successive differentiation of the DE, and becomes restricted if the DE has singularities anywhere in the complex  $z$  plane.

Holubec and Stauffer (1985) have proposed a way around this problem based on the idea of analytically continuing a Frobenius series rather than a Taylor series. The method is applied to second-order linear DE with a regular singularity and with analytic coefficients which are finite polynomials. In practice the method works for arbitrary order and for more general analytic coefficients. The technique was originally applied to second-order linear DE of the form

$$u'' + P(z)u' + Q(z)u = 0 \quad (5)$$

with  $P(z)$  and  $Q(z)$  finite polynomials. However, it can also be adapted to more general equations (Hodgson 1988b).

Potentials of the form (1) or (3) can be easily handled with this procedure, as the DE takes the form

$$u'' + Q(z)u = 0 \quad (6)$$

with

$$Q(z) = E - V(z). \quad (7)$$

The general solution  $u$  is expanded in a Taylor series about the point  $z_0$  as

$$u = \sum_{i=0}^{N_i} c_i (z - z_0)^i. \quad (8)$$

The polynomial coefficient  $Q(z)$  must be expanded in a similar manner:

$$Q(z) = \sum_{i=0}^q \tilde{Q}_i (z - z_0)^i. \quad (9)$$

By substituting these expansions for  $u(z)$  and for  $Q(z)$  into the DE, and by setting the coefficients of the different powers of  $(z - z_0)$  to zero, we arrive at a set of recurrence relations to generate the coefficients  $c_i$ .

For the potential form (3) the complete expansion for  $Q(z)$  becomes

$$Q(z) = (E - V_0) + 6V_0z_0^2 - 3V_0z_0^4 + 12V_0z_0(1 - z_0^2)(z - z_0) + 6V_0(1 - 3z_0^2)(z - z_0)^2 - 12V_0z_0(z - z_0)^3 - 3V_0(z - z_0)^4 \quad (10)$$

where  $V_0 = 200$ . These lead to the general recurrence relation for the  $c_i$  coefficients:

$$(k+2)(k+1)c_{k+2} + \sum_{i=0}^4 \tilde{Q}_i c_{k-i} = 0 \quad (11)$$

which is valid for  $k \geq 0$  with the understanding that  $c_k = 0$  if  $k < 0$ . The initial values  $c_0 = u(z_0)$  and  $c_1 = u'(z_0)$  are used to start the series.

If we start from the origin, we can use the above results with  $z_0 = 0$ . In the general case a Frobenius series is used, with the appropriate characteristic exponent. For the oscillator problem under examination here the characteristic exponent is 0, and so the regular Taylor series about  $z_0 = 0$  suffices.

The initial conditions chosen at the boundary  $z = 0$  must be such that the generated wavefunction is either even or odd, since parity is preserved by this potential. Selecting  $u(0) = c$  and  $u'(0) = 0$  generates an even parity wavefunction, corresponding to the ground state, and every other energy level. Similarly, by selecting  $u(0) = 0$  and  $u'(0) = c$ , odd parity functions are generated. Here  $c$  is an arbitrary normalisation constant.

The numerical procedure is based on a finite interval on the  $z$  axis,  $0 < z < R$ . The eigenvalues are then computed by dividing this range into  $N_s$  equal intervals of length  $h$ . A Taylor series is generated about the origin ( $z_0 = 0$ ), and is used to compute the values of the function and its derivative at  $z = h$ . Then  $z_0$  is set equal to  $h$  and the series (8) is used to calculate the wavefunction and its derivative at  $2h$ . This process continues out to  $z = R$ , employing an initial guess for the eigenvalue  $E$ . The value of  $E$  is then adjusted and the process repeated until the value of the wavefunction at  $R$  is as close to zero as is possible within the precision of the calculations.

The process is initiated by locating two values of  $E$  which lie on either side of the correct eigenvalue, such that they produce values of the wavefunction at  $R$  having opposite signs. The secant method is then used to generate a new guess for  $E$ :

$$E^{i+1} = E^i - u^i(R) \frac{E^i - E^{i-1}}{u^i(R) - u^{i-1}(R)}. \quad (12)$$

Here  $u(z)$  represents the wavefunction, and the superscripts indicate the order of iteration. In practice, 7-10 iterations are required to achieve the precision presented below.

Application of this approach to potential (1) is effectively using what Chaudhuri and Mukherjee (1984) refer to as the finite-box approximation. The potential is unbounded in  $x$ , and must satisfy the boundary condition that the wavefunction vanish at  $\pm\infty$ . It has been found that the lower eigenvalues are unaffected by replacing this

with the condition that the wavefunction vanish at a finite  $R$ . This does not apply to potential (3) as it is defined to be infinite at the boundary,  $x = \pm 2$ .

### 3. Results and discussion

As a general remark, we note that the degree of accuracy (i.e. the number of significant figures) in the eigenvalues that we have been able to obtain by our method appears to diminish slowly with the increase in quantum numbers. Also the accuracy possible is usually greater for odd-parity levels than for even-parity levels. Higher accuracies can be achieved at the expense of greater computation times. The higher energy levels require that the range  $R$  be increased, with a consequent increase in the number of intervals.

In table 1 we compare the results obtained by our procedure for the potential (1) with those obtained by Balsa *et al* (1983) for certain values of  $k$  when  $\lambda = 1$ . As  $k$  increases, the magnitude of the splitting decreases. Generally speaking, the agreement between our values and those of Balsa *et al* (1983) is very good. Some fine points, however, may be noted. For  $k = 50$ , Balsa *et al* found  $E_0$  and  $E_1$  to be the same to 12 significant figures. Our more accurate results show that the splitting shows up at the 21st significant figure. For the same value of  $k$ , Balsa *et al* found  $E_{38}$  and  $E_{39}$  to differ at the eleventh significant figure. Our results show that the two are identical to at least 17 significant figures.

**Table 1.** Eigenvalues for the double-well anharmonic oscillator of (1): (a) present study, (b) Balsa *et al* (1983).

		$k = 5.0, \lambda = 1$	$k = 50.0, \lambda = 1$
$E_0$	a	-3.410 142 761 239 83	-615.020 090 902 757 816 566 22
	b	-3.410 142 761 24	-615.020 090 903
$E_1$	a	-3.250 675 362 289 236	-615.020 090 902 757 816 565 01
	b	-3.250 675 362 29	-615.020 090 903
$E_{20}$	a	96.101 737 842 7	-422.068 788 468 852
	b	96.101 737 842 7	-422.068 788 469
$E_{38}$	a	244.366 964 364 5	-261.112 800 996 988 49
	b	244.366 964 365	-261.112 800 997
$E_{39}$	a	253.583 300 287 527	-261.112 800 996 988 49
	b	253.583 300 288	-261.112 800 987

Next we consider the potential (3). Our results, along with those of wo and Talman (1980), are shown in table 2. The eigenvalues quoted from wo are those computed using the bisection method with extrapolation. It will be noticed that our results are quite close to those of wo but differ significantly from those of Talman (1980). The splitting increases rapidly as one goes to higher levels. Our values for  $(E_1 - E_0)$ ,  $(E_3 - E_2)$  and  $(E_5 - E_4)$  are  $9.8195 \times 10^{-12}$ ,  $3.3856 \times 10^{-9}$  and  $5.19 \times 10^{-16}$  respectively. At this point we wish to note a puzzling fact. While the individual eigenvalues of Talman differ from ours in the fifth, fourth and third significant place for these three pairs, the splittings are surprisingly close to our values. Talman's data give the following values for these three splittings:  $11.7 \times 10^{-12}$ ,  $3.7575 \times 10^{-9}$  and  $5.419 935 \times 10^{-6}$ . We have no simple explanation for this situation.

**Table 2.** Energies for the double-minimum potential of (3): (a) present study, (b) Wolniewicz and Orlikowski (1978), (c) Talman (1980).

$E_0$	a	-751.522 312 383 846 149
	b	-751.522 312 1
	c	-751.580 510 591 922 8
$E_1$	a	-751.522 312 383 836 329 544
	b	-751.522 311 6
	c	-751.580 510 591 911 1
$E_2$	a	-656.713 389 223 403
	b	-656.713 391 2
	c	-656.988 966 447 361 6
$E_3$	a	-656.713 389 220 017 445 27
	b	-656.713 389 8
	c	-656.988 966 443 604 1
$E_4$	a	-565.390 612 802
	c	-566.063 380 018 952 1
$E_5$	a	-565.390 612 283 166 5
	c	-566.063 379 476 958 6

#### 4. Conclusions

The analytic continuation procedure of Holubec and Stauffer (1985) offers a straightforward solution to the problem of obtaining high-accuracy wavefunctions and eigenvalues for Schrödinger's equation, even for potentials such as the double-minimum potentials considered here where the eigenvalues are almost degenerate.

#### Acknowledgment

This research was supported in part by a research grant from NSERC held by one of the authors (YPV).

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