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Perturbation theory for the triple-well anharmonic oscillator

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Abstract. We study perturbation theory at large order for the one-dimensional Schrödinger equation with the potential $U(x)=x^2(R^2-x^2)^2/8R^4$, where R is a large parameter. It is shown that for the states which 'originate' from the middle well, in addition to the Rayleigh–Schrödinger expansion of the energy eigenvalues in power series of $1/R^2$ there is an exponentially small shift in R^2 due to the tunnelling into the side wells. The states which 'belong' to the side wells exhibit asymptotic eigenvalue degeneracy. Non-modal solutions for these states are also found, and by using them we determine the large-k behaviour of the general kth Rayleigh–Schrödinger coefficient. The comparison of asymptotic formulae with the results of numerical calculations shows an excellent agreement where it is expected.

1. Introduction

This paper is concerned with the nature of Rayleigh–Schrödinger perturbation theory for the triple-well anharmonic oscillator described by the Schrödinger equation

$$\mathrm{d}^2\psi/\mathrm{d}x^2+[2E-x^2(R^2-x^2)^2/4R^4]\psi=0. \tag{1}$$

We assume that R is a large parameter. The potential $U(x)=x^2(R^2-x^2)^2/8R^4$ has three minima at $x=0$, $x=\pm R$. The boundary condition $\lim_{|x|\to\infty}\psi(x)=0$ selects out a discrete set of energy eigenvalues E which naturally is subdivided into two subsets. We refer to them later as states I and states II. States I 'originate' from the middle well at $x=0$. Their energy eigenvalues E can be approximated by the perturbation expansion

$$E=\tfrac{1}{2}n+\tfrac{1}{4}+\sum_{k=1}E_k/R^{2k}. \tag{2}$$

States II 'originate' from two degenerate wells centred at $x=\pm R$. Corresponding energy eigenvalues E_{g} and E_{u} possess double-well character

$$E_0=\tfrac{1}{2}(E_{\mathrm{g}}+E_{\mathrm{u}})=n'+\tfrac{1}{2}+\sum_{k=1}E'_k/R^{2k}. \tag{3}$$

The symbols n and n' in (2) and (3) denote positive integers or zeros. The coefficients E_k and E'_k can be found by using standard perturbation theory.

In our paper we consider two problems which, as will be seen later on, are closely connected.

First, we obtain the exponentially small corrections to the energy eigenvalues defined by Rayleigh–Schrödinger expansions (2) and (3), i.e. terms which vanish more rapidly than any power $(R)^{-2k}$ as R^{-2} tends to zero. For states II the meaning of such a correction is well known—it gives the energy eigenvalue splitting $\Delta E = E_g - E_u$, whereas for states I it represents an energy shift δE which should be added to the expansion (1) to improve the asymptotic value of E.

Second, we determine the large-k behaviour of the coefficients E_k and E'_k. This problem has been widely discussed. For a comprehensive review the reader may consult the article of Simon (1982).

We present in detail the procedure for the states I. For states II only the results we obtained are quoted.

Recently, equation (1) was studied as a part of a more general problem by Benassi *et al* (1979). In particular, these authors (Benassi *et al* 1979) have obtained numerical results for the non-modal solution of equation (1) for the 'ground state' resonance. The comparison of our results with those of Benassi *et al* (1979) will be given.

It is important to mention that the problem considered is essentially different from those where potentials have only two identical wells, i.e. double-well problems. This remark applies to both states I and states II. The peculiarity arises from the need to account for the particle tunnelling into the well, which is not identical with that one where the particle is located.

2. States I

Due to the symmetry of the problem with respect to the sign of x it is sufficient to find the solution of equation (1) for $x \geqslant 0$. Our solution scheme is based on dividing the x axis into three regions:

$$\begin{array}{ll} \text{Region I} & 0 \leqslant x \ll R. \\ \text{Region II} & |\eta| < 1, \text{ where } \eta = x/R. \\ \text{Region III} & |q| \ll R, \text{ where } q = R - x. \end{array} \tag{4}$$

After the solutions in these regions are found, we link them together; taking into account the boundary condition, we deduce the eigenfunction of equation (1).

2.1. Region I

Substituting the new function

$$\psi = \exp(-\tfrac{1}{4}x^2 + x^4/8R^2)\varphi(x) \tag{5}$$

into (1), we obtain the following equation for φ:

$$\frac{d^2\varphi}{dx^2} - x\frac{d\varphi}{dx} + (2E - \tfrac{1}{2})\varphi = -\frac{1}{R^2}\left(x^3\frac{d\varphi}{dx} + \tfrac{3}{2}x^2\varphi\right). \tag{6}$$

In zero order of $1/R^2$, $E = \frac{1}{2}n + \frac{1}{4}$, where n is a quantum number. Except for $n = 0$, n does not coincide with the number of the state of equation (1) since there are states II where the particle is located at $x = \pm R$.

For symmetrical states I (even n) the solution of equation (6) can be obtained as

$$\varphi = \sum_{k=0} \frac{1}{R^{2k}}\varphi_k(x), \qquad \varphi_k(x) = \sum_{s=-2k}^{k} a_s^{(k)} F(-\tfrac{1}{2}n - s; \tfrac{1}{2}; \tfrac{1}{2}x^2), \tag{7}$$

where E is taken in the form (2), and $F(a;c;y)$ is a confluent hypergeometric function. $a_s^{(k)}$ and E_k are to be determined from recurrence relations which follow from (6):

$$sa_s^{(k)}=\sum_{j=0}^{k-1}E_{k-j}a_s^{(j)}-\tfrac{1}{2}(n+2s-\tfrac{1}{2})(n+2s-1)a_{s-1}^{(k-1)}$$
$$+\tfrac{3}{2}[(n+2s)(n+2s+1)+\tfrac{1}{2}]a_s^{(k-1)}-\tfrac{3}{2}(n+2s+\tfrac{3}{2})(n+2s+2)a_{s+1}^{(k-1)}$$
$$+\tfrac{1}{2}(n+2s+2)(n+2s+4)a_{s+2}^{(k-1)},\qquad a_s^{(0)}=\delta_{s0}. \tag{8}$$

In the first power of $1/R^2$ we obtain $a_{-2}^{(1)}=-\frac{1}{2}n(\frac{1}{2}n-1)$, $a_{-1}^{(1)}=\frac{3}{2}n(n-\frac{1}{2})$, $a_1^{(1)}=-\frac{1}{2}(n+1)(n+\frac{3}{2})$; $a_0^{(1)}$ is an arbitrary constant and we take it equal to zero,

$$E_0=\tfrac{1}{2}n+\tfrac{1}{4}-(6n^2+6n+3)/4R^2+\mathrm{O}(R^{-4}). \tag{9}$$

If one is interested only in the Rayleigh–Schrödinger expansion (2) for E_0 then it is sufficient to have relation (8). But we show that expansion (2) is not quite satisfactory as an asymptotic formula for E. An exponentially small shift δE should be added in order to make the asymptotic expansion for E more consistent, i.e. we need $E=E_0+\delta E$. In order to perform our task we used the procedure elaborated by us earlier (Damburg and Propin 1968a, b, 1971, 1974). The essential part of this procedure consists in the substitution $n\to n+\lambda$ where λ is an exponentially small value which is characteristic for different problems. In order to find λ we need solutions of equation (1) for regions II and III. In principle, finding λ and consequently δE expanded in powers of $1/R^2$ can be reduced to a system of recurrence relations. But we limit our consideration to terms up to the order of $1/R^2$.

2.2. *Region II*

The equation for φ_1 here can be written as

$$\eta(1-\eta^2)\mathrm{d}\varphi_1/\mathrm{d}\eta+[-2E-1+\tfrac{3}{2}(1-\eta^2)]\varphi_1=R^{-2}\mathrm{d}^2\varphi_1/\mathrm{d}\eta^2. \tag{10}$$

Taking into account (9), we obtain

$$\psi_1=\exp[R^2(-\tfrac{1}{4}\eta^2+\tfrac{1}{8}\eta^4)]\varphi_1(\eta)$$
$$=D_1\exp[R^2(-\tfrac{1}{4}\eta^2+\tfrac{1}{8}\eta^4)]\frac{\eta^n}{(1-\eta^2)^{n/2+3/4}}$$
$$\times\left[1+\frac{1}{R^2}\left(C_1^{(1)}-\frac{n(n-1)}{2\eta^2(1-\eta^2)^2}+\frac{12n^2+12n+21}{16(1-\eta^2)^2}\right.\right.$$
$$\left.\left.+\frac{6n^2+6n+3}{4(1-\eta^2)}\right)+\mathrm{O}(R^{-4})\right]. \tag{11}$$

Similarly, we can find the second solution of equation (1) for the region II,

$$\psi_2=D_2\exp[R^2(\tfrac{1}{4}\eta^2-\tfrac{1}{8}\eta^4)]\frac{(1-\eta^2)^{n/2-1/4}}{\eta^{n+1}}\left[1+\frac{1}{R^2}\left(C_2^{(1)}+\frac{(n+1)(n+2)}{2\eta^2(1-\eta^2)^2}\right.\right.$$
$$\left.\left.-\frac{12n^2+12n+21}{16(1-\eta^2)^2}-\frac{6n^2+6n+3}{4(1-\eta^2)}\right)+\mathrm{O}(R^{-4})\right]. \tag{12}$$

In (11) and (12) $D_1, D_2, C_1^{(1)}$ and $C_2^{(1)}$ are constants which have to be determined by the linking procedure performed in the region $1\ll x\ll R$.

2.3. Region III

For the function φ_1 we have for this region the equation

$$\frac{d^2\varphi_1}{dq^2}+2q\frac{d\varphi_1}{dq}+(2E+1)\varphi_1=\frac{1}{R}\left(3q^2\frac{d\varphi_1}{dq}+3q\varphi_1\right)-\frac{1}{R^2}\left(q^3\frac{d\varphi_1}{dq}+\tfrac{3}{2}q^2\varphi_1\right). \tag{13}$$

With accuracy up to the terms of $O(R^{-3})$ we find

$$\begin{aligned}\psi_1=A\exp\left(-\tfrac{1}{2}q^2+\frac{1}{2R}q^3-\frac{1}{8R^2}q^4\right)\{&F(-\tfrac{1}{4}n+\tfrac{1}{8};\tfrac{1}{2};q^2)\\&+R^{-1}[b_0^{(0)}qF(-\tfrac{1}{4}n+\tfrac{1}{8};\tfrac{3}{2};q^2)+b_{-1}^{(0)}qF(-\tfrac{1}{4}n+\tfrac{9}{8};\tfrac{3}{2};q^2)\\&+b_{-2}^{(0)}qF(-\tfrac{1}{4}n+\tfrac{17}{8};\tfrac{3}{2};q^2)]+R^{-2}[d_1^{(1)}F(-\tfrac{1}{4}n-\tfrac{7}{8};\tfrac{1}{2};q^2)\\&+d_0^{(1)}F(-\tfrac{1}{4}n+\tfrac{1}{8};\tfrac{1}{2};q^2)+d_{-1}^{(1)}F(-\tfrac{1}{4}n+\tfrac{9}{8};\tfrac{1}{2};q^2)\\&+d_{-2}^{(1)}F(-\tfrac{1}{4}n+\tfrac{17}{8};\tfrac{1}{2};q^2)+d_{-3}^{(1)}F(-\tfrac{1}{4}n+\tfrac{25}{8};\tfrac{1}{2};q^2)]\}\end{aligned} \tag{14}$$

where

$$\begin{aligned}&b_0^{(0)}=\tfrac{3}{8}(n+\tfrac{3}{2})^2, \qquad b_{-1}^{(0)}=\tfrac{3}{4}(n-\tfrac{1}{2})^2, \qquad b_{-2}^{(0)}=-\tfrac{1}{8}(n-\tfrac{1}{2})(n-\tfrac{9}{2}),\\&d_1^{(1)}=-\tfrac{1}{128}(n+\tfrac{3}{2})(9n^2+41n+\tfrac{149}{4}), \qquad d_{-1}^{(1)}=-\tfrac{15}{128}(n-\tfrac{1}{2})(2n^2-10n+\tfrac{9}{2}),\\&d_{-2}^{(1)}=\tfrac{1}{64}(n-\tfrac{1}{2})(n-\tfrac{9}{2})(6n-11), \qquad d_{-3}^{(1)}=-\tfrac{1}{128}(n-\tfrac{1}{2})(n-\tfrac{9}{2})(n-\tfrac{17}{2}).\end{aligned} \tag{15}$$

Constants A and $d_0^{(1)}$ are to be determined by the linking procedure in the region $1\ll q\ll R$. The second fundamental solution ψ_2 of equation (1) for region III can be obtained if in (14) the following substitutions are made:

$$F(a;c;y)\to F(a;c;y)-\frac{\Gamma(c)\Gamma(a-c+1)}{\Gamma(a)\Gamma(2-c)}y^{1-c}F(a-c+1;2-c;y). \tag{16}$$

So, in the zero order of $1/R$, ψ_2 in region III can be presented as

$$\psi_2=B\exp(-\tfrac{1}{2}q^2)\left(F(-\tfrac{1}{4}n+\tfrac{1}{8};\tfrac{1}{2};q^2)-\frac{2\Gamma(-\tfrac{1}{4}n+\tfrac{5}{8})}{\Gamma(-\tfrac{1}{4}n+\tfrac{1}{8})}qF(-\tfrac{1}{4}n+\tfrac{5}{8};\tfrac{3}{2};q^2)\right). \tag{17}$$

2.4. Linking procedure

In order to avoid writing out cumbersome expressions we limit our considerations still more by keeping to the zero order of $1/R$. By using formulae given above, it is easy to extend our derivation up to the next order, i.e. up to the terms $\sim 1/R^2$.

As we noted above we should first make the substitution $n\to n+\lambda$ (λ being exponentially small) in (7). After such substitution and corresponding expansion in powers of λ are performed (as described by Damburg and Propin (1971)), we get for the region $1\ll x\ll R$

$$\begin{aligned}\psi=(-1)^{n/2}&\frac{2^{-n/2}\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}n+\frac{1}{2})}x^n\exp(-\tfrac{1}{4}x^2)[1+O(x^{-2})]\\&+(-1)^{n/2+1}\lambda\Gamma(\tfrac{1}{2})\Gamma(\tfrac{1}{2}n+1)2^{n/2-1/2}x^{-n-1}\exp(\tfrac{1}{4}x^2)[1+O(x^{-2})].\end{aligned} \tag{18}$$

For the same region $1 \ll x \ll R$ for functions ψ_1 and ψ_2 defined by (11) and (12) we obtain

$$\psi_1 = D_1 R^{-n} x^n \exp(-\tfrac{1}{4}x^2)[1+O(x^{-2})],$$
$$\psi_2 = D_2 R^{n+1} x^{-n-1} \exp(\tfrac{1}{4}x^2)[1+O(x^{-2})]. \tag{19}$$

Therefore,

$$D_1 = (-1)^{n/2} \frac{\Gamma(\frac{1}{2})R^n}{2^{n/2}\Gamma(\frac{1}{2}n+\frac{1}{2})}, \qquad D_2 = (-1)^{n/2+1} \frac{\Gamma(\frac{1}{2})\Gamma(\frac{1}{2}n+1)2^{n/2-1/2}}{R^{n+1}} \lambda. \tag{20}$$

The total function for the region II is

$$\psi = \psi_1 + \psi_2. \tag{21}$$

Consider now the linking region $1 \ll q \ll R$. Here for functions (11) and (12) we get

$$\psi_1 = D_1 \frac{R^{n/2+3/4}}{2^{n/2+3/4}} \exp(-\tfrac{1}{8}R^2) q^{-n/2-3/4} \exp(\tfrac{1}{2}q^2)[1+O(q^{-2})], \tag{22}$$

$$\psi_2 = D_2 \frac{2^{n/2-1/4}}{R^{n/2-1/4}} \exp(\tfrac{1}{8}R^2) q^{n/2-1/4} \exp(-\tfrac{1}{2}q^2)[1+O(q^{-2})]. \tag{23}$$

Similarly by considering formulae (14) and (17),

$$\psi_1 = A \frac{\Gamma(\frac{1}{2})}{\Gamma(-\frac{1}{4}n+\frac{1}{8})} q^{-n/2-3/4} \exp(\tfrac{1}{2}q^2)[1+O(q^{-2})], \tag{24}$$

$$\psi_2 = -B \frac{\Gamma(-\frac{1}{4}n+\frac{5}{8})}{\sqrt{2\pi}} q^{n/2-1/4} \exp(-\tfrac{1}{2}q^2)[1+O(q^{-2})]. \tag{25}$$

Comparing (22), (23) and (24), (25), we determine A and express B through λ. Finally, it is necessary to choose the proper asymptotic behaviour for $\psi = \psi_1 + \psi_2$ at $q \to -\infty$ (i.e. $x \to \infty$). The function ψ should decrease exponentially and this requirement yields $A = -2B$. As a result we obtain

$$\lambda = \lambda_0[1 + \kappa_1/R^2 + O(R^{-4})],$$
$$\lambda_0 = -\frac{R^{3n+3/2}}{2^{n/2+1/4}\Gamma(\frac{1}{2}n+\frac{3}{4})\Gamma(n+1)} \exp(-\tfrac{1}{4}R^2), \qquad \kappa_1 = -\tfrac{1}{8}(72n^2+72n+39). \tag{26}$$

Formula (26) is obtained for even n. For odd n, the corresponding formula differs from (26) only in sign, i.e. $\lambda_0 \to -\lambda_0$. Now we determine the energy shift δE by substituting in (2) $n+\lambda$ instead of n, and after expanding $E_0(n+\lambda)$ in powers of λ retaining terms of the first order of λ. So we get $E = E_0 + \delta E$ where

$$E_0 = \tfrac{1}{2}n + \tfrac{1}{4} - (6n^2+6n+3)/4R^2 + O(R^{-4}),$$
$$\delta E = (-1)^{n+1} \frac{R^{3n+3/2}\exp(-\frac{1}{4}R^2)}{2^{n/2+5/4}\Gamma(\frac{1}{2}n+\frac{3}{4})\Gamma(n+1)} \left(1 - \frac{72n^2+120n+63}{8R^2} + O(R^{-4})\right). \tag{27}$$

2.5. *'Level width' and the large-k behaviour of E_k*

Due to the fact that the first indices in the confluent hypergeometric functions in (17) are fractional, the function (17) has different branches at $q \to \infty$. Choosing instead of (25)

$$\psi_2 = \mathrm{i}B\frac{\Gamma(-\frac{1}{4}n+\frac{5}{8})}{\sqrt{2\pi}}q^{n/2-1/4}\exp(-\tfrac{1}{2}q^2)[1+\mathrm{O}(q^{-2})], \tag{28}$$

we obtain as a result the non-modal asymptotic solution of equation (1) considered recently by Benassi *et al* (1979), where

$$E = E_0+\tfrac{1}{2}\mathrm{i}\gamma, \qquad \gamma = 2|\delta E|. \tag{29}$$

E_0 is determined as previously by (2). Benassi *et al* (1979), relying upon intuition, had presented the leading term for γ for the 'ground state'. The expression given by them has correct exponent by incorrect pre-exponential multiplier.

After we have obtained the non-modal solution of equation (1) and consequently γ, we can derive the large-k behaviour for coefficients E_k in (2) by applying the procedure proposed by Bender and Wu (1973) and Simon (1970, 1982):

$$\begin{aligned} E_k &= -\frac{1}{2\pi}\int_0^\infty \rho^{k-1}\gamma(\rho)\,\mathrm{d}\rho \\ &= -\frac{2^{2k+n/52+1/4}}{\pi\Gamma(n+1)\Gamma(\frac{1}{2}n+\frac{3}{4})}\Gamma(k+\tfrac{3}{2}n+\tfrac{3}{4})\left(1-\frac{72n^2+120n+63}{32(k+\frac{3}{2}n-\frac{1}{4})}+\mathrm{O}(k^{-2})\right). \end{aligned} \tag{30}$$

2.6. *Comparison with the results of numerical calculations*

We have solved equation (1) numerically for different values of R for the ground and the first excited states. In addition, by using recurrence relations (8), exact values of the coefficients E_k were determined. These coefficients are necessary both for the calculations of asymptotic values of E_0 by using (2) and for comparison with formula (30).

In table 1, the numerical results of Benassi *et al* (1979) for the 'ground state' resonance of equation (1) are also given. They correspond, as mentioned earlier, to our non-modal solution at $n = 0$.

In table 2, results for the first excited state are presented. According to formula (27), E has different sign for odd and even n; this is seen from tables 1 and 2.

When calculating E_0 from the Rayleigh–Schrödinger expansion (2), we invoked a standard rule for asymptotic expansions, terminating just before the term smallest in magnitude. The first omitted term by order of magnitude is equal to the intrinsic error of the expansion (2).

In all cases considered the error was essentially smaller than $|\delta E|$, and with the increasing of R the ratio of the error to $|\delta E|$ was decreasing. Thus, the necessity to bring in δE when calculating $E = E_0+\delta E$ is established not only on the basis of theoretical consideration, but is also confirmed numerically.

As mentioned above, the error in calculating $E = E_0+\delta E$ is decreasing when R is increasing. At the same time, it is seen from table 2 that the value $\delta E = E_{\mathrm{num}} - E_0$ has slightly uneven behaviour when R is increasing. The explanation is evident: the number of terms taken for calculation of E_0 is increased by jumps whereas R is increasing gradually.

Table 1. $n = 0$.

$g = \sqrt{2}/R$	E_{num}	E'†	E, formula (2) E_0	N‡	First discarded term in (2)
0.20	0.233 119 073	0.233 138 944	0.233 1397	11	0.44×10^{-5}
0.22	0.228 671 492	0.228 813 420	0.228 8090	9	0.34×10^{-4}
0.24	0.223 010 610	0.223 605 098	0.223 6203	7	0.16×10^{-3}
0.26	0.215 847 272	0.217 528 843	0.217 8898	6	0.51×10^{-3}
0.28	0.207 294 077	0.210 833 623	0.210 3548	6	0.125×10^{-2}
0.30	0.197 918 128	0.203 901 962	0.203 3179	4	0.25×10^{-2}

$g = \sqrt{2}/R$	$\delta E = E = E_{num} - E'$	$\frac{1}{2}\gamma$†	One term, formula (27)	Two terms, formula (27)
0.20	$-0.198\,71 \times 10^{-4}$	$0.197\,70 \times 10^{-4}$	$0.240\,43 \times 10^{-4}$	$0.202\,56 \times 10^{-4}$
0.22	$-0.141\,93 \times 10^{-3}$	$0.142\,61 \times 10^{-3}$	$0.182\,41 \times 10^{-3}$	$0.147\,51 \times 10^{-3}$
0.24	$-0.594\,49 \times 10^{-3}$	$0.606\,15 \times 10^{-3}$	$0.833\,6 \times 10^{-3}$	$0.644\,5 \times 10^{-3}$
0.26	$-0.168\,16 \times 10^{-2}$	$0.177\,60 \times 10^{-2}$	$0.267\,0 \times 10^{-2}$	$0.195\,9 \times 10^{-2}$
0.28	$-0.353\,95 \times 10^{-2}$	$0.397\,9 \times 10^{-2}$	$0.662\,0 \times 10^{-2}$	$0.457\,5 \times 10^{-2}$
0.30	$-0.598\,38 \times 10^{-2}$	$0.735\,0 \times 10^{-2}$	1.357×10^{-2}	$0.876\,3 \times 10^{-2}$

† Data of Benassi *et al* (1979), who adopted different notations in equation (1). Their value of E is four times larger than ours. We use in table 1 our present notations. The value of g is introduced to make a more convenient comparison of our results with those of Benassi *et al* (1979).
‡ N is the number of terms taken into account in formula (2).

Table 2. $n = 1$.

R	E_{num}	E_0	N†	$E_{num} - E_0$	δE, formula (27), one term	δE, formula (27), two terms
7	0.654 974 699	0.651 148 4	9	0.3826×10^{-2}	0.9971×10^{-2}	$0{\cdot}3485 \times 10^{-2}$
8	0.681 034 189	0.680 827 34	13	0.2068×10^{-3}	0.4276×10^{-3}	0.2146×10^{-3}
9	0.697 941 260	0.697 934 854	18	0.6406×10^{-5}	1.036×10^{-5}	0.6283×10^{-5}
10	0.708 987 349	0.708 987 249	23	1.00×10^{-7}	1.4405×10^{-7}	0.9813×10^{-7}

† N is the number of terms taken into account in formula (2).

Another numerical test for our asymptotic formulae can give us the comparison of the results obtained by using formula (30) with the exact values of coefficients E_k. Results are presented in tables 3–5.

Table 3. Ground state, $n = 0$.

k	Formula (30), leading term	Formula (30), two terms	$E_{k,num}$
10	$-0.654\,86 \times 10^{12}$	$-0.522\,63 \times 10^{12}$	$-0.499\,05 \times 10^{12}$
20	$-0.388\,92 \times 10^{30}$	$-0.350\,15 \times 10^{30}$	$-0.347\,95 \times 10^{30}$
50	$-0.447\,04 \times 10^{94}$	$-0.429\,35 \times 10^{94}$	$-0.429\,03 \times 10^{94}$
70	$-0.178\,06 \times 10^{142}$	$-0.173\,04 \times 10^{142}$	$-0.172\,975 \times 10^{142}$

Table 4. $n = 1$.

k	Formula (30), leading term	Formula (30), two terms	$E_{k,\mathrm{num}}$
10	$-1.825\,98\times10^{14}$	$-0.532\,58\times10^{14}$	$-0.627\,72\times10^{14}$
20	$-0.286\,19\times10^{33}$	$-0.178\,87\times10^{33}$	$-0.182\,29\times10^{33}$
50	$-0.124\,51\times10^{98}$	$-0.105\,15\times10^{98}$	$-0.105\,50\times10^{98}$
70	$-0.814\,69\times10^{145}$	$-0.723\,57\times10^{145}$	$-0.724\,76\times10^{145}$

Table 5. $n = 2$.

k	Formula (30), leading term	Formula (30), two terms	$E_{k,\mathrm{num}}$
20	$-0.851\,88\times10^{35}$	$-0.160\,31\times10^{35}$	$-0.296\,02\times10^{35}$
30	$-0.274\,48\times10^{56}$	$-0.119\,69\times10^{56}$	$-0.141\,71\times10^{56}$
60	$-0.615\,51\times10^{124}$	$-0.434\,35\times10^{124}$	$-0.448\,14\times10^{124}$
70	$-0.140\,29\times10^{149}$	$-0.104\,67\times10^{149}$	$-0.107\,02\times10^{149}$

2.7. *One application of asymptotic formula (30)*

There is supposition (Simon 1982) that the study of large-k behaviour of E_k can provide a key to the problem of summability of asymptotically diverging Rayleigh–Schrödinger expansions similar to (2). We would like to indicate here another application of formula (30).

When applying formula (2) for E_0, we terminated the series just before the smallest term. The question arises as to how many terms we should keep then in formula (27) for δE when calculating $E = E_0 + \delta E$. It is clear that all terms in (27) for δE which are smaller in magnitude than the first term discarded in (2) are meaningless. From (30) it is easy to estimate the maximum value of R where the second term in (27) becomes smaller than the intrinsic error of (2). From

$$E_{k_m}/(E_{k_m-1}R^2) \approx 1 \tag{31}$$

we find

$$k_m \approx \tfrac{1}{4}R^2 - \tfrac{3}{2}n + \tfrac{1}{4}. \tag{32}$$

Therefore, the intrinsic error of (2) by order of magnitude is

$$\left|\frac{E_{k_m}}{R^{2k_m}}\right| \sim \frac{2^{-n/2+1/4}R^{3n+1/2}}{\sqrt{\pi}\,\Gamma(n+1)\Gamma(\frac{1}{2}n+\frac{3}{4})}\exp(-\tfrac{1}{4}R^2)\left(1 - \frac{72n^2+120n+63}{8R^2}\right). \tag{33}$$

The ratio of the second term in (27) to (33) becomes smaller than 1 at

$$R > \frac{\sqrt{\pi}}{2^{3/2}}\,\frac{72n^2+120n+63}{8}\left(1 + \frac{64}{\pi(72n^2+120n+63)}\right). \tag{34}$$

From (34) it follows that at $n = 0$, $R > 6.5$ and at $n = 1$, $R > 22$. As can be seen from table 1, this estimate is in full agreement with numerical data.

We were discussing above the use of formula (27) for δE in the calculation $E = E_0 + \delta E$. But the value δE itself can be found numerically with much higher accuracy; then, comparing δE with formula (27), all decreasing terms in (27) (we have calculated only two of them) can be accounted for except, as a general rule, in asymptotic expansions, the last one. Such a value of δE can be obtained if one calculates the difference between the numerical energy eigenvalues E for modal and non-modal solutions of equation (1) for the same state. An example is given in table 1 for $n=0$. It is a remarkable fact that we have here a situation quite similar to that encountered in the symmetrical double-well problem when calculating $\Delta E = E_g - E_u$.

3. States II

The procedure of finding asymptotic solutions for this case is similar and was presented by us earlier (Damburg and Propin 1974). However, in order to make this article more complete we quote here the results obtained:

$$E = E_0 \pm \tfrac{1}{2}\Delta E, \qquad E_0 = n + \tfrac{1}{2} + \sum_{k=1} \frac{1}{R^{2k}} E'_k, \tag{35}$$

$$\Delta E = \frac{2^{3n+1}}{\sqrt{2\pi}} \frac{\Gamma(2n+1)}{\Gamma(n+1)\Gamma(4n+2)} R^{6n+3} \exp(-\tfrac{1}{4}R^2)[1 + \mathrm{O}(R^{-2})].$$

For $n=0$ we found the next term for ΔE to be

$$\Delta E = \sqrt{2/\pi} R^3 \exp(-\tfrac{1}{4}R^2)[1 - 141/8R^2 + \mathrm{O}(R^{-4})]. \tag{36}$$

Comparison of formula (36) with exact numerical data shows that at $R=6$, (36) gives an error ~18% and at $R = 12.5$ an error ~0.1%.

In the above-mentioned paper (Damburg and Propin 1974), non-modal solutions for the states II were not considered. Quite similarly to the previously considered case, the solutions are given by the expression

$$E = E_0 + \tfrac{1}{2}\mathrm{i}\gamma \tag{37}$$

where $\gamma = \Delta E$.

With γ we find the large-k behaviour for E'_k:

$$E'_k = -\frac{2^{k+6n+3/2}}{\pi} \frac{\Gamma(2n+1)(6n+2k+1)!!}{\Gamma(n+1)\Gamma(4n+2)} [1 + \mathrm{O}(k^{-1})]. \tag{38}$$

For $n=0$,

$$E'_k = -(2^{k+3/2}/\pi)(2k+1)!![1 - 141/16(2k+1) + \mathrm{O}(k^{-2})]. \tag{39}$$

Comparison of (39) with the exact numerical values of E'_k is presented in table 6.

Table 6. Ground state, $n=0$.

k	Formula (35), leading term	Formula (35), two terms	$E_{k,\mathrm{num}}$
10	$-1.267\,58 \times 10^{13}$	$-0.735\,65 \times 10^{13}$	$-0.694\,25 \times 10^{13}$
20	$-1.237\,94 \times 10^{31}$	$-0.971\,86 \times 10^{31}$	$-0.965\,22 \times 10^{31}$
30	$-0.172\,28 \times 10^{52}$	$-0.147\,39 \times 10^{52}$	$-0.147\,12 \times 10^{52}$
40	$-0.639\,68 \times 10^{73}$	$-0.570\,08 \times 10^{73}$	$-0.569\,59 \times 10^{73}$

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