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Large-order perturbation theory for the O(2) anharmonic oscillator with negative anharmonicity and for the double-well potential

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Abstract. For the O(2) anharmonic oscillator with negative anharmonicity and one-dimensional double-well potential $U(x)=(x^2-R^2)^2/8R^2$, R is a large parameter for both problems, conventional Rayleigh–Schrödinger expansions in power series of $1/R^2$ for the energy eigenvalues agree. We studied asymptotic expansions for the eigenvalues which contain, in addition to the perturbation series, exponentially small terms in R^2 due to the tunnelling through corresponding potential barriers. Numerical calculations are also performed and comparisons with the asymptotic formulae are given.

1. Introduction

The phenomenon of quantum-mechanical tunnelling continues to be a subject of active study because of its many areas of application and because of its intrinsic interest. This phenomenon is the cause for the presence of exponentially small terms in the energy eigenvalue in addition to the perturbation series. As it was shown (Bender and Wu 1973, Simon 1970, 1982), the large-order behaviour of the perturbation series for the anharmonic oscillator with negative anharmonicity depends on the imaginary part of the energy, i.e. on exponentially small terms. The situation with double wells appeared to be much more complicated (Simon 1982).

The authors of the present paper started a study of double wells in the late sixties. Two problems were considered: the molecular ion H_2^+, including the oblate spheroidal equation (Damburg and Propin 1968a, b) and the Schrödinger equation for the one-dimensional double-well potential $U(x)=(x^2-R^2)^2/8R^2$ (Damburg and Propin 1971). At that time we limited our study to the exponentially small terms of the lowest order, namely, for the double-well potential, by the terms $\sim\exp(-\frac{2}{3}R^2)$. We obtained a system of recurrence relations which allowed us to determine the exact coefficients of the 'perturbation' series for the energy $E_{\rm pt}$ and for the level splitting $\Delta E=E_u-E_g$ for arbitrary powers of $1/R^2$ and for any state. In the present paper, based on the earlier results, we continue the study of the double-well potential $U(x)$ and combine with it the consideration of the closely connected problem of the O(2) anharmonic oscillator with negative anharmonicity. The computer calculations show that the perturbation series for the energy for the double well in one dimension and for the

O(2) anharmonic oscillator with negative anharmonicity agree (Seznec and Zinn-Justin 1979, Avron and Seiler 1981).

The exponentially small terms which are present in asymptotic expansions of the eigenvalues in both problems are proportional to the different powers of the value $\sim\exp(-\frac{2}{3}R^2)$. A partial study of the meaning of such terms was undertaken by us earlier (Damburg and Propin 1983). We derived the asymptotic formula in K for the coefficients b_K of expansion in powers of $1/R^2$ for the level width Γ. Here we continue to examine other exponentially small terms. Some preliminary ideas on the problem were presented by Damburg and Propin (1982) earlier. A different approach to the problem considered in this paper was elaborated by Zinn-Justin (1981b, 1982, 1984) who, besides others, discussed the question of the summation of the perturbation series. The scope of the problems raised in our paper is essentially different.

2. Double well. Preliminaries

We consider the one-dimensional Schrödinger equation

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+\frac{(x^2-R^2)^2}{8R^2}\right)\Psi_{g,u}=E_{g,u}\Psi_{g,u}. \tag{1}$$

The potential $(x^2-R^2)^2/8R^2$ has two minima at $x=\pm R$. We assume that R is a large parameter. Owing to the symmetry of the problem with respect to the sign of x, there are two sets of solutions of equation (1): odds and evens with the energies

$$E_{g,u}=E_0\mp\tfrac{1}{2}\Delta E.$$

In our present approach to the asymptotic solution of equation (1) we essentially rely upon the method and results we obtained previously (Damburg and Propin 1971). We start from the conventional Rayleigh–Schrödinger perturbation theory and find the eigenvalue in the form of the expansion

$$\begin{aligned}E_{\text{pt}}&=\sum_{K=0}E_K R^{-2K}\\&=n+\tfrac{1}{2}-\frac{3n^2+3n+1}{4R^2}-\frac{34n^3+51n^2+35n+9}{32R^4}\\&\quad-\frac{375n^4+750n^3+792n^2+417n+89}{128R^6}-\dots\end{aligned} \tag{2}$$

where n is a positive integer or zero.

Formula (2) for the eigenvalue $E_{g,u}$ is an unsatisfactory one since a conventional perturbation expansion does not allow us to account for exponentially small terms which arise because of particle tunnelling through a potential barrier and, first of all, the level splitting $\Delta E=E_u-E_g$. To overcome the inadequacy of the perturbation expansion, we make the substitution $n\to n+\alpha(n)$ where $\alpha\sim\exp(-\frac{2}{3}R^2)$, into (2) and into corresponding expansions of wavefunctions $\Psi_{g,u}$. The value $\alpha(n)$ is determined by matching solutions of equation (1) obtained for different regions of x. As a result, we obtain a system of recurrence relations which allows us to determine $\alpha(n)$ in the form of the expansion in power series in $1/R^2$. We should note, however, that there are two algebraic errors in the recurrence relations in the paper by Damburg and Propin (1971). For convenience we present the improved formulae in the appendix.

The leading term obtained earlier for ΔE is correct, while the second term in the expansion of ΔE in powers of $1/R^2$ is correct only for the ground state $n=0$.

Below we just present the corrected and extended results for $\alpha_{g,u}$ obtained by the procedure mentioned (Damburg and Propin 1971)

$$\alpha_{g,u} = \mp\alpha_0 \sum_{K=0} \kappa_K/R^{2K}, \qquad \kappa_0 = 1, \tag{3}$$

$$\alpha_0 = \frac{2^{3n+1}R^{2n+1}}{\sqrt{\pi}\,\Gamma(n+1)} e^{-\frac{2}{3}R^2}, \tag{4}$$

$$\kappa_1 = -(102n^2+102n+35)/48,$$

$$\kappa_2 = (10\,404n^4+2808n^3-9456n^2-11\,868n-3779)/2(48)^2, \tag{5}$$

$$\kappa_3 = (1/(48)^4)(-8489\,664n^6+18\,595\,008n^5+14\,383\,008n^4$$
$$-21\,358\,080n^3-6307\,3584n^2-46\,010\,448n-11\,733\,688).$$

The formulae (2)–(5) are necessary for the present study.

After α is found, we can determine the level splitting in the lowest order of α_0

$$\Delta\varepsilon = 2\alpha_u \frac{dE_{pt}}{dn} = 2\alpha_0 \sum_{K=0} \frac{1}{R^{2K}} \sum_{j=0}^{K} \frac{dE_j}{dn} \kappa_{K-j}$$
$$= 2\alpha_0 \sum_{K=0} a_K/R^{2K}. \tag{6}$$

We retain the notation ΔE for the total difference

$$E_u - E_g = \Delta E = \Delta\varepsilon + O(\alpha_0^3).$$

To avoid cumbersome expressions, we only present below results for $n=0$. By using formulae (2)–(5), it is quite easy to obtain results for arbitrary n.

3. The O(2) anharmonic oscillator with negative anharmonicity

The Schrödinger equation can be written as

$$(-y\, d^2/dy^2 - 1/4y + y/4 - y^2/8R^2 - E)\phi(y) = 0, \qquad 0 \leqslant y < \infty. \tag{7}$$

By using the conventional perturbation theory, one can get the following expansion for E:

$$E_{pt} = \sum_{K=0} \frac{E_K}{R^{2K}}, \qquad E_0 = n + \tfrac{1}{2}. \tag{8}$$

Seznec and Zinn-Justin (1979) numerically computed 60 coefficients E_K for $n=0$ of expansions (2) and (8) and found that they agreed with an accuracy of at least 12 places and to all orders computed. This observation was 'sharpened and extended' by Avron and Seiler (1981) who showed that the agreement holds analytically for all states at least up to 11th order. However, the strict proof of the identity of (2) and (8) was not given. Our observation on the identity of (2) and (8) is more fundamental.

One of the recurrence relations for the double well, which allows us to find the coresonding E_K (Damburg and Propin 1971, formula (17)) is

$$\begin{aligned} 2sd_s^{(K)} &= \tfrac{1}{4}(n+s+1)(n+s+2)d_{s+2}^{(K-1)} \\ &\quad + (n+s+1)^2 d_{s+1}^{(K-1)} + \tfrac{1}{2}[3(n+s)(n+s+1)+1]d_s^{(K-1)} \\ &\quad + (n+s)^2 d_{s-1}^{(K-1)} + \tfrac{1}{4}(n+s)(n+s-1)d_{s-2}^{(K-1)} + 2\sum_{j=0}^{K-1} E_{K-j} d_s^{(j)}, \\ d_0^{(0)} &= 1, \qquad E_0 = n + \tfrac{1}{2}, \qquad -2K \leqslant s \leqslant 2K, \end{aligned} \tag{9}$$

where K and s are integers.

The recurrence relation for E_K for the O(2) anharmonic oscillator with negative anharmonicity is exactly the same. It can be seen from formula (37) of the paper by Damburg and Kolosov (1983) where it is necessary to put $m = 0$ and to make the obvious substitutions $C_K^{(j)} = (-1)^{K+j} 2^j d_K^{(j)}$ and $\lambda_1^{(K)} = (-1)^K 2^K E_K$. Therefore, E_K in (2) and (8) agree for all n and K. However, from this fact, as was correctly noted by Seznec and Zinn-Justin (1979), the equality of the values $E_c = (E_g + E_u)/2$ and Re E^{osc} does not follow. One of the aims of our paper is to study the function

$$f(E) = E_c - \operatorname{Re} E^{\text{osc}}. \tag{10}$$

4. Double well. Corrections $\sim\alpha_0^2$ and α_0^3

As we noted in the introduction, we aim to obtain in asymptotic expansions of $E_{g,u}$, terms which are proportional to the powers of the value $\alpha_0 \sim \exp(-\frac{2}{3}R^2)$. To perform this task, we match again, this time more thoroughly, solutions of equation (1) obtained for two different regions of x in the region $1 \ll R - x \ll R$ where both solutions are valid. The necessary expressions are given in our previous article (Damburg and Propin 1971). The result can be represented by the expression

$$\sin(\pi\alpha_{g,u}) = \pi(-1)^{\alpha_{g,u}(n)}\alpha_{g,u}(n) \tag{11}$$

where the function $\alpha_{g,u}(n)$ is defined by formulae (3)–(5). In the first power of α_0 formula (11) naturally comes to the identity $\alpha_{g,u} = \alpha_{g,u}$.

The number n in formula (11) should be treated as the procedure

$$n \to n + \alpha_{g,u}(n + \alpha_{g,u}(n + \ldots)\ldots). \tag{12}$$

The terms containing different powers of α_0 in $\alpha_{g,u}$ can be determined in an elementary way by using formulae (3)–(5), (11) and (12) by expansion in α_0. Finally, to obtain $E_{g,u}$ we use formula (2) for E_{pt}, in which we substitute $n + \alpha_{g,u}$ instead of n and again, where it is necessary, expand the obtained expression in powers of α_0.

$$E_{g,u} = E_{\text{pt}} \mp \tfrac{1}{2}\Delta\varepsilon + \delta E + \tfrac{1}{2}\mathrm{i}\gamma \mp \tfrac{1}{2}\delta\varepsilon - \tfrac{1}{2}\mathrm{i}\delta\gamma \tag{13}$$

where

$$\gamma = 2\pi\alpha_{g,u}^2 \frac{\mathrm{d}E_{\text{pt}}}{\mathrm{d}n} = 2\pi\alpha_0^2 \sum_{K=0} \frac{b_K}{R^{2K}}, \tag{14}$$

$$\delta E = \frac{\gamma}{2\pi}[2\ln R + 3\ln 2 - \psi(1)] - \frac{\alpha_0^2}{R^2}\left(\frac{23}{8} - \frac{13}{192\,R^2} + \frac{45\,941}{9216\,R^4} + \ldots\right), \tag{15}$$

$$\delta\varepsilon = 2\alpha_0^3\left[\{\tfrac{3}{2}[2\ln R + 3\ln 2 - \psi(1)]^2 - \tfrac{17}{12}\pi^2\}\left(1 - \frac{47}{16R^2} - \frac{163}{512R^4} - \frac{89\,635}{24\,576R^6} - \ldots\right)\right.$$
$$-[2\ln R + 3\ln 2 - \psi(1)]\left(\frac{63}{8R^2} - \frac{825}{128R^4} + \frac{24483}{4096R^6} - \ldots\right)$$
$$\left.-\frac{17}{8R^2} + \frac{297}{32R^4} - \frac{194\,801}{12\,288R^6} + \ldots\right], \tag{16}$$

$$\delta\gamma = 2\pi\alpha_0^3\left[3[2\ln R + 3\ln 2 - \psi(1)]\left(1 - \frac{47}{16R^2} - \frac{163}{512R^4} - \frac{89\,635}{24\,576R^6} - \ldots\right)\right.$$
$$\left.-\frac{63}{8R^2} + \frac{825}{128R^4} - \frac{24\,483}{4096R^6} + \ldots\right]. \tag{17}$$

Coefficients b_K can be easily computed by using the formulae for $\alpha_{g,u}$ and E_{pt}. We do not present them since they agree exactly with the coefficients calculated by Silverstone *et al* (1981) for the similar expansion of Γ for the O(2) anharmonic oscillator with negative anharmonicity. Moreover, we have an equality

$$\Gamma = \gamma + O(\alpha_0^4). \tag{18}$$

5. The application of the asymptotic formulae obtained

The problems of the double well and the O(2) anharmonic oscillator with negative anharmonicity can be solved numerically. We compare the numerical (exact) data with the results obtained by the asymptotic formulae. Formula (13) for $E_{g,u}$ contains terms of different powers of α_0. It is more convenient to split formula (13) into two, the first of which would contain only even powers of α_0, the second only odd:

$$E_c = \tfrac{1}{2}(E_g + E_u) = E_{pt} + \delta E + \tfrac{1}{2}i\gamma + O(\alpha_0^4), \tag{19}$$

$$\Delta E = E_u - E_g = \Delta\varepsilon + \delta\varepsilon - \tfrac{1}{2}i\delta\gamma + O(\alpha_0^5). \tag{20}$$

In the present paper we compare asymptotic formulae with the numerical solution of equation (1) for the modal case, i.e. for the case where the imaginary part of E is absent. It corresponds to

$$E_{c,\mathrm{mod}} = E_{pt} + \delta E + O(\alpha_0^4), \tag{21}$$

$$\Delta E_{\mathrm{mod}} = \Delta\varepsilon + \delta\varepsilon + O(\alpha_0^5). \tag{22}$$

We note that numerical data for the solutions of equation (1) which we are able to find in the literature always correspond to the modal case. Having in mind this case, we henceforth omit the index 'mod' in formulae. We shall consider non-modal numerical solutions of equation (1) in our next paper.

The asymptotic series in powers of $1/R^2$ for E_{pt} and $\Delta\varepsilon$ are divergent and so do not allow us to calculate these quantities exactly. Therefore, the natural question arises: are the exponentially small quantities δE and $\delta\varepsilon$ in formulae (21) and (22) meaningful values or not? We would be able to answer this question if there were explicit expressions for the coefficients E_K and a_K for arbitrary K, but this problem cannot easily be solved. However, it is possible to obtain asymptotic formulae in K for E_K and a_K, which would allow us to estimate the term smallest in magnitude in expansions E_{pt} and $\Delta\varepsilon/2\alpha_0$ in powers of $1/R^2$ for chosen R which is large. We proceed in the spirit of the paper by Bender and Wu (1973) but without strict mathematical foundation. The mathematical validity of the similar approach is proved in the paper by Damburg *et al* (1984).

In order to derive the dispersion relation for coefficients E_K, we should know the analytical properties of the function $E_c(R^2)$ for whole R^2 complex plane (Bender and Wu 1973). We simply assume that $E_c(R^2)$ is analytic in the whole R^2 complex plane except one branch cut running from +0 to $+\infty$, where we have found its asymptotic form (19). We assume also that for all R^2, except the real R^2 axis from +0 to $+\infty$, the asymptotic expansion of $E_c(R^2)$ agrees with E_{pt}. With these assumptions we can use for the calculation of the coefficients E_K the same formulae which are given in the paper by Bender and Wu (1973):

$$\begin{aligned} E_K &= -\frac{1}{2\pi}\int_0^\infty (R^2)^{K-1}\gamma(R^2)\,\mathrm{d}(R^2) \\ &= -\frac{4}{\pi}\left(\frac{3}{4}\right)^{K+1}\Gamma(K+1)\sum_{j=0}\left(\frac{4}{3}\right)^j\frac{\Gamma(K-j+1)}{\Gamma(K+1)}b_j. \end{aligned} \tag{23}$$

By using quite similar assumptions we obtain a formula for a_K, asymptotic in K

$$\begin{aligned} a_k &= -\frac{1}{2\pi}\int_0^\infty (R^2)^{K-1}\frac{\delta\gamma(R^2)}{2\alpha_0}\,\mathrm{d}(R^2) \\ &= -\frac{9}{\pi}\left(\frac{3}{4}\right)^{K}\Gamma(K+1)\left[A+\frac{B}{K}+\frac{C}{K(K-1)}+\frac{D}{K(K-1)(K-2)}+\cdots\right], \end{aligned} \tag{24}$$

where

$$\begin{aligned} A &= \psi(K+1)+\ln 6-\psi(1), \\ B &= -\{47[\psi(K)+\ln 6-\psi(1)]+42\}/12, \\ C &= -\{163[\psi(K-1)+\ln 6-\psi(1)]-1100\}/288, \\ D &= -\{89\,635[\psi(K-2)+\ln 6-\psi(1)]+48\,966\}/10\,368. \end{aligned} \tag{25}$$

Later we show how to improve formulae asymptotic in K, for E_K. In table 1, we compare the results for a_K obtained by using asymptotic formula (24) with exact values, which we also obtained by using the recurrence relations obtained earlier (Damburg and Propin 1971).

Table 1. Accuracy of the asymptotic formula (24) for a_K.

K	$a_{K,\mathrm{num}}$	$a_{K,\mathrm{as}}$
12	-1.2877×10^{8}	-1.3074×10^{8}
14	-1.4926×10^{10}	-5050×10^{10}
20	-9.1886×10^{16}	-9.2029×10^{16}
22	$-2.497\,33\times10^{19}$	$-2.499\,56\times10^{19}$

The first two terms of formula (24), i.e. coefficients A and B, agree with the similar result presented by Zinn-Justin (1981a), who at first 'guessed' that A and B had a form $S_K = c_K \ln K + d_K$ and then applied the Neville procedure for the numerical analysis of 94 terms of the 'perturbation' expansion of $\Delta\varepsilon/2\alpha_0$.

6. Intrinsic error in the asymptotic expansions for E_c and ΔE

It is known that for the alternating asymptotic series the highest accuracy is achieved when the series is terminated just before the term which is smallest in magnitude. The error of the sum in such cases does not exceed in magnitude the first discarded term (Gradshteyn and Ryzhik 1965). We have supposed that the same rule is valid for the asymptotic series which arise in the double-well problem, though all the terms in the series here have the same sign.

As we have already determined the large-K behaviour of coefficients E_K, we are able to estimate the value of the smallest term in expansion E_{pt} for the fixed but large enough R^2

$$\omega = (E_K/R^{2K})_{\min} = -(3/2\pi)^{1/2} 4R\, e^{-\frac{4}{3}R^2}[1-(31/12R^2)+O(R^{-4})]. \tag{26}$$

Comparison of (26) and (15) shows that the leading term of δE essentially exceeds intrinsic error of E_{pt} and, therefore, δE should be taken into account in calculations of E_c by formula (21).

Similarly we can find the intrinsic error for the asymptotic expansion of $\Delta\varepsilon$:

$$\omega' = -3(6\pi)^{1/2}(\alpha_0^3/R)[2\ln R + 3\ln 2 - \psi(1) + O(\ln R/R^2)] \tag{27}$$

and, consequently, come to the conclusion that in the calculation of ΔE using formula (22), the term $\delta\varepsilon$ should be taken into account. The terms $\sim\alpha_0^4$ etc at any R, where the asymptotic expansion for E_c is meaningful, are essentially smaller than ω and, therefore, should not be taken into account. Similarly, the terms $\sim\alpha_0^5$ etc are meaningless in calculations of ΔE. When asymptotic formulae are used for calculations of E_g and E_u, there is no need to take into account the terms $\sim\alpha_0^3$ (in contrast to the case of $\Delta E = E_u - E_g$!).

7. The calculation of $f(E)$

As was mentioned above, the level width Γ of the O(2) anharmonic oscillator with negative anharmonicity and γ for double-well potential are connected by formula (18) $\Gamma = \gamma + O(\alpha_0^4) \sim \alpha_0^2$. Therefore, in the asymptotic expansion of E^{osc} the real exponentially small term $\sim\Gamma^2 \sim \alpha_0^4$ (Damburg and Propin 1983) and consequently

$$f(E) = E_c - \mathrm{Re}\, E^{\mathrm{osc}} = \delta E + O(\alpha_0^4). \tag{28}$$

If we calculate E_c and Re E^{osc} separately by using asymptotic formulae, then the terms $\sim\alpha_0^4$ are meaningless. But when we calculate $f(E)$, then in the asymptotic expansion of δE after we have taken into account all terms which are larger than the smallest one, we should include also some terms which are $\sim\alpha_0^4$. However, the calculation of many terms in the asymptotic expansion of δE is a difficult algebraic problem which we would not tackle.

8. Comparison of numerical data with the results obtained by asymptotic formulae

In order to compare asymptotic formulae with the 'exact' results, we solved numerically equations (1) and (7) by using the known methods (see for example Damburg and Kolosov 1983). We computed E_g, E_u, Re E^{osc} and Γ for different values of R^2. By use of the necessary recurrence relations we also calculated numerical (exact) values of the coefficients E_K and a_K for large enough K. We were also using the exact values of the coefficients b_K calculated by Silverstone *et al* (1981). In tables 2 and 3, we present comparisons.

Table 2. Comparison of exact values of E_c and Re E^{osc} with perturbation value E_{pt}.

R	$E_{c,num}$	Re E^{osc}_{num}	E_{pt}, formula (2)			ω, formula (26)
			E_{pt}	N	ω_{num}	
2.6	0.454 130 198	0.451 673 034	0.451 578 719	7	-0.51×10^{-3}	-0.54×10^{-3}
3.0	0.467 156 216	0.466 931 404	0.466 937 330	10	-0.37×10^{-4}	-0.36×10^{-4}
3.2	0.471 858 273	0.471 804 231	0.471 803 728	13	-0.78×10^{-5}	-0.78×10^{-5}
3.6	0.478 577 160	0.478 575 068	0.478 574 991	17	-0.25×10^{-6}	-0.25×10^{-6}
4.0	0.483 053 433	0.483 053 384	0.483 053 390	21	-0.51×10^{-8}	-0.51×10^{-8}

N is the number of terms taken into account in formula (2). ω_{num} is the value of the smallest term in (2) which is not taken into account in the calculation of E_{pt}.

Table 3. Comparison of exact values $f(E)$ with δE.

R	$f(E)_{num}$	δE, formula (15)†
2.6	0.2457×10^{-2}	0.2583×10^{-2}
3.0	0.2248×10^{-3}	0.2284×10^{-3}
3.2	0.5404×10^{-4}	0.5447×10^{-4}
3.6	0.2092×10^{-5}	0.2097×10^{-5}
4.0	0.49×10^{-7}	0.495×10^{-7}

† In formula (15) terms $\sim\alpha_0^2 \ln R/R^8$ etc were not taken into account.

From the data presented in tables 2 and 3, it is clear that the theoretical conclusions stated above are fully justified:

(1) The value Re E^{osc} with asymptotic accuracy can be represented by E_{pt}.

(2) To obtain E_c, the value δE should be added to E_{pt}.

(3) In both cases the error of calculation does not exceed the magnitude of the smallest term of the expansion (8), which is not taken into account in the calculation of E_{pt}. Similar comparisons for ΔE are given in table 4:

Table 4. Exact values $\Delta E/2\alpha_0$ and their asymptotic counterparts.

R	$\Delta E_{num}/2\alpha_0$	$\Delta\varepsilon/2\alpha_0$	N	$\delta\varepsilon/2\alpha_0$	$\omega'_{num}/2\alpha_0$
3.0	0.807 181 09	0.806 742 96	10	0.000 714 83	−0.000 416
3.2	0.835 4079	0.835 2610	12	0.000 1955	−0.000 0968
3.6	0.874 8207	0.874 8128	16	0.000 009 08	−0.000 003 48
3.8	0.889 041	0.889 039	18	0.000 001 59	−0.000 000 546

N is the number of terms in (6) used for calculation of $\Delta\varepsilon$. ω'_{num} is the value of the smallest term in (6) which is not taken into account in the calculation of $\Delta\varepsilon$.

It is seen from table 4 that in all cases the difference $|\Delta E_{\rm num} - \Delta\varepsilon| > |\omega'|$. At the same time $|\Delta E_{\rm num} - (\Delta\varepsilon + \delta\varepsilon)| < |\omega'|$.

Thus, in table 4, we give a numerical illustration of the presence of the terms $\sim\alpha_0^3$ in the asymptotic expansion for ΔE.

9. Multiple power exponential terms in the O(2) anharmonic oscillator with negative anharmonicity

As we have already mentioned (Damburg and Propin 1983), in order to obtain the exponentially small terms in the asymptotic expansion for E for the equation (7), we can use the same procedure which has been used for the double-well potential. Consequently, in $E_{\rm pt}$ and in corresponding expansions of the wavefunction, we use the substitution $n \to n + {\rm i}\lambda$, $\lambda \sim \alpha_0^2 \sim \exp(-\frac{4}{3}R^2)$. As a result, we obtain

$$\begin{aligned} E &= E_{\rm pt} + \tfrac{1}{2}{\rm i}\Gamma + {\rm O}(\lambda^2), \\ \Gamma &= 2\lambda\ {\rm d}E_{\rm pt}/{\rm d}n + {\rm O}(\lambda^2) = 2\pi\alpha_0^2 \sum_{K=0} b_K/R^{2K} + {\rm O}(\lambda^2). \end{aligned} \tag{29}$$

To obtain the exponentially small terms $\sim\lambda^2$ (terms in higher powers of λ appear to be less than the intrinsic errors in the asymptotic expansions considered below), it is necessary to use the relation

$$\lambda = (-1)^{2\lambda(n)}\lambda(n + {\rm i}\lambda(n)), \tag{30}$$

which similarly to the relation (11) represents the result of the matching of the solutions of equation (7) obtained for different regions of y.

We considered earlier the real term $\sim\lambda^2$ and by using it derived formulae asymptotic in K for the coefficients b_K (Damburg and Propin 1983). The imaginary term $\sim\lambda^2$ produces a correction to the level width Γ:

$$\begin{aligned} \Gamma_{\rm as} &= 2(\lambda - 2\pi\lambda^2)\,{\rm d}E_{\rm pt}/{\rm d}n = \Gamma_1 + \Gamma_2 \\ &= 8R^2\,{\rm e}^{-\frac{4}{3}R^2} \sum_{K=0} \frac{b_K}{R^{2K}} - 64\pi R^4\,{\rm e}^{-\frac{8}{3}R^2}\left(1 - \frac{11}{3R^2} + \frac{289}{288R^4} - \frac{66697}{20736}R^6 + \ldots\right). \end{aligned} \tag{31}$$

By using the formula for b_K, asymptotic in K, obtained earlier it is easy to check that for large R, $|\Gamma_2/\Gamma_1^{\rm min}| \sim R/\ln R$, where $\Gamma_1^{\rm min}$ is the smallest term of the first sum. Therefore, strictly speaking, in the formula (31) it is necessary to take into account both terms. Some comparisons are given in table 5.

As can be seen from table 5, the difference $\Gamma_{\rm num} - \Gamma_{\rm as}$ is smaller in magnitude than the $|\Gamma_1^{\rm min}|$, but this is not true for the difference $\Gamma_{\rm num} - \Gamma_1$. The terms which are $\sim\lambda^2$

Table 5. Accuracy of asymptotic formula (31) for Γ.

R	$\Gamma_{\rm num}$	Γ_1	N	Γ_2	$\Gamma_{\rm as} = \Gamma_1 + \Gamma_2$	$\Gamma_1^{\rm min}$
2.6	$0.400\,07 \times 10^{-2}$	$0.405\,15 \times 10^{-2}$	7	-0.639×10^{-4}	$0.398\,76 \times 10^{-2}$	-0.365×10^{-4}
3.0	$0.321\,686 \times 10^{-3}$	$0.322\,156 \times 10^{-3}$	10	-0.369×10^{-6}	$0.321\,787 \times 10^{-3}$	-0.221×10^{-6}
3.2	$0.737\,910 \times 10^{-4}$	$0.738\,140 \times 10^{-4}$	12	-0.189×10^{-7}	$0.737\,951 \times 10^{-4}$	-0.114×10^{-7}
3.6	$0.266\,006 \times 10^{-5}$	$0.266\,0088 \times 10^{-5}$	16	-0.238×10^{-10}	$0.266\,0064 \times 10^{-5}$	-0.141×10^{-10}

N is the number of terms which are taken into account in first sum of (31).

should also be taken into account in determining the large-K behaviour of E_K. Inserting the value $\Gamma_1+\Gamma_2$ in (23) instead of γ, we obtain

$$E_K=-\frac{4}{\pi}\left(\frac{3}{4}\right)^{K+1}\Gamma(K+1)\left(\sum_{j=0}\left(\frac{4}{3}\right)^j\frac{\Gamma(K-j+1)}{\Gamma(K+1)}b_j+A_K\right),$$

$$A_K=-\frac{3\pi(K+1)}{2^{K+1}}\left(1-\frac{88}{9(K+1)}+\frac{578}{81(K+1)K}-\frac{133\,394}{2187(K+1)K(K-1)}+\ldots\right). \tag{32}$$

As was noted above, E_K for the O(2) anharmonic oscillator with negative anharmonicity agrees exactly with E_K for the double-well potential. In order to obtain the second series in (32) and in the derivation strictly confining to the 'boundaries' of the double-well problem, one would need to consider in formula (19) the terms $\sim\alpha_0^4$.

However, it would be difficult to separate such terms from the terms of the same order $\sim\alpha_0^4$, which are 'responsible' for the large-K behaviour of the coefficients in expansion in power series of $1/R^2$ of the value $\delta E/\alpha_0^2$. But it is clear that performing the task, we would come inevitably to the same result, i.e. to formula (32).

Table 6 provides comparisons with numerical data for E_K, where

$$E_K^{(0)}=-\frac{4}{\pi}\left(\frac{3}{4}\right)^{K+1}\Gamma(K+1), \qquad B_K=\sum_{j=0}\left(\frac{4}{3}\right)^j\frac{\Gamma(K-j+1)}{\Gamma(K+1)}b_j.$$

As can be seen from table 6, the difference $E_{K,\mathrm{num}}/E_K^{(0)}-E_{K,\mathrm{as}}/E_K^{(0)}$ is less in magnitude than the smallest term in B_K (this term has not been taken into account in the calculation of $E_{K,\mathrm{as}}$). At very large K, the value of A_K becomes essentially larger than many terms in the vicinity of the term smallest in magnitude, B_K. However, it would be difficult to confirm this statement by numerical data since it would require calculations of E_K at $K\sim10^3$–10^4 to many significant figures.

Table 6. Exact values $E_{K,\mathrm{num}}/E_K^{(0)}$ and their asymptotic counterparts.

K	$E_{K,\mathrm{num}}/E_K^{(0)}$	B_K	N	A_K	The smallest term in B_K
15	0.786 265	0.787 168	7	-0.921×10^{-3}	-0.825×10^{-3}
20	0.845 181 9	0.845 267 8	9	-0.513×10^{-4}	-0.446×10^{-4}
25	0.877 943 30	0.877 946 57	12	-0.230×10^{-5}	-0.199×10^{-5}
30	0.899 071 999 6	0.899 072 102 0	15	-0.939×10^{-7}	-0.808×10^{-7}

10. Conclusion

In the present paper the role of different powers of exponentially small terms in the asymptotic expansion of energy was considered for the first time. These terms are due to quantum-mechanical tunnelling. It is shown how to use them to determine the large-K behaviour of the Kth coefficient of the 'perturbation expansion' for E_{pt}, ΔE, Γ etc. It is also shown that in calculations using asymptotic formulae, the highest accuracy can be achieved only if corresponding exponentially small terms (if they exist) are taken into account. However, we should emphasise that the main motivation for our investiagation was not the elaboration of the asymptotic procedure for obtaining numerical values E_c, ΔE, Γ etc. The problems considered can be easily solved by direct numerical methods. Our aim was the study of the nature of the perturbation theory of large order.

Appendix

The corrected expressions for formulae (18*b*) and (27*b*) of the paper by Damburg and Propin (1971) are:

$$d_0^{(K)} = \sum_{s=1}^{K} (-1)^s 2^s \frac{\Gamma(n+2s+1)(2s-1)!!}{\Gamma(2s+1)\Gamma(n+1)} a_s^{(K)} - \sum_{s=1}^{\min(n,2K)} \frac{\Gamma(n+1)}{\Gamma(n-s+1)\Gamma(s+1)} d_{-s}^{(K)}. \tag{18b}$$

$$\kappa_K = \sum_{t=0}^{2K} \frac{(\frac{8}{3})^t}{\Gamma(t+1)} \sum_{s=3t}^{2(K+t)} (-1)^s \frac{\Gamma(n+s+1)}{\Gamma(s-3t+1)\Gamma(n+3t+1)} d_s^{(k+t)}$$
$$- \sum_{t=1}^{K} \kappa_{K-t} \sum_{s=1}^{3t} \frac{1}{4^s\Gamma(s+1)} a_{-s}^{(t)}. \tag{27b}$$

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