

## Energy levels of the quartic double well using a phase-integral method

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Approximate energy eigenvalues for the double-well quartic oscillator are calculated using the phase-integral method of Fröman and Fröman up to the fifth-order approximation. By means of appropriate transformations, the integrals appearing in the quantization condition are expressed in terms of integrals solved in previous papers. Different approximations are discussed. In general, the results are very good.

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### I. INTRODUCTION

Double-well potentials appear often in physics and have been a subject of permanent interest over the years from both the classical and the quantum points of view. For quantum double-well potentials, a great variety of methods have been implemented to study their eigenvalues and other properties (see, e.g., Ref. [1] and references therein). Among these quantum double wells, the most studied [2] is the quartic,

$$V(z) = v_2 z^2 + v_4 z^4, \quad (1.1)$$

where  $v_2 < 0$  and  $v_4 > 0$ . This is not an easy problem: the perturbation expansion of the eigenvalues  $\mathcal{E}_n(v_2, v_4)$  in powers of  $v_4$  is divergent [3], and the variational methods are not devoid of difficulties [4].

An old and well-known approximation able to deal with the quartic double-well is the JWKB method to first order [5–7]. This procedure is equivalent to the phase-integral method of Fröman and Fröman of first order [8]. But for higher-order approximations, this last method is, for several reasons [9,10], preferable to the JWKB method. These reasons are related to the appropriate handling of the wave-function connection problem and the lack of flexibility of the higher-order JWKB method in dealing with cases where approximate solutions of the Schrödinger equation over the whole range of the independent variable are unsatisfactory. Lakshmanan, Karlsson, and Fröman [11], for the quartic single well [Eq. (1.1) with  $v_2 > 0$  and  $v_4 > 0$ ], were able to evaluate in terms of elliptic integrals the integrals appearing in the first four terms of a generalized Bohr-Sommerfeld (GBS) rule of seventh order deduced from the phase-integral method, and thereby achieve great numerical precision in calculating the eigenvalues of this well. Also, recently Yuste [12] has evaluated in terms of elliptic integrals the integrals appearing in the GBS rule to ninth order for the quartic double barrier [Eq. (1.1) with  $v_2 > 0$  and  $v_4 < 0$ ] and for the quartic double well. For this last case, the rule used only gave the *unsplit* energy levels, i.e., the energy levels calculated assuming that the internal barrier between the two wells is totally opaque. When the barrier is large enough, this assumption is good, and the results obtained from the GBS rule are excellent, competing in precision and ease of calculation with the varia-

tional methods. However, when the barrier is thin or the energy levels are close to the top of the barrier, the approximation is no longer valid and the GBS results are poor.

The purpose of the present work is to express the quartic double-well phase-integral quantification conditions of Fröman and Fröman up to fifth order [13–15] in terms of complete elliptic integrals in order to make these conditions very well adapted for numerical evaluation of the energy levels of the quartic double well, taking into consideration the splitting and shifting due to the internal barrier. By means of appropriate transformations all relevant integrals appearing in these quantization conditions are expressed in terms of integrals already evaluated in Refs. [11] and [12].

The structure of the paper is as follows. Section II gives a short presentation of the phase-integral method and quantization conditions of Fröman and Fröman for double wells up to the fifth order. The integrals appearing in this quantization condition for the quartic double well with energies below the internal barrier peak (sub-barrier case) are explicitly solved in terms of complete elliptic integrals in Sec. III. The same is done in Sec. IV for energies above the barrier peak (superbarrier case). In Sec. V we check our results against published values, discussing their goodness in different cases. In Sec. VI some concluding remarks are given.

### II. PHASE-INTEGRAL METHOD APPLIED TO DOUBLE WELLS

In this section we summarize the phase-integral method of Fröman and Fröman [8] and present the quantization condition for double wells given by Fröman *et al.* [15]. In the phase-integral method of Fröman and Fröman, the exact solution of the one-dimensional Schrödinger equation

$$\frac{d^2\psi}{dz^2} + R(z)\psi = 0, \quad (2.1)$$

with

$$R(z) = \frac{2\mu}{\hbar^2} [\mathcal{E} - V(z)], \quad (2.2)$$

is written as

$$\psi(z) = q^{-1/2} \exp \left[ \pm i \int^z q(z) dz \right]. \quad (2.3)$$

Consequently  $q(z)$  must satisfy

$$q^{-3/2} \frac{d^2}{dz^2} q^{-1/2} + R(z)/q^2 - 1 = 0. \quad (2.4)$$

Let  $Q(z)$  be an approximate solution of (2.4). Then

$$\epsilon_0 = Q^{-3/2}(z) \frac{d^2}{dz^2} Q^{-1/2}(z) + \frac{R(z) - Q^2(z)}{Q^2(z)} \quad (2.5)$$

will be small compared with unity. Writing  $q(z)$  as

$$q(z) = Q(z)g(z), \quad (2.6)$$

$g(z)$  can be expressed as an asymptotic series [8,16]:

$$g(z) = \sum_{j=0}^N Y_{2j}, \quad (2.7)$$

where

$$Y_0 = Z_0, \quad (2.8a)$$

$$Y_2 = Z_2, \quad (2.8b)$$

$$Y_4 = Z_4 - \frac{1}{8} \frac{d^2 \epsilon_0}{d\xi^2}, \quad (2.8c)$$

⋮

with

$$Z_0 = 1, \quad (2.9a)$$

$$Z_2 = \frac{1}{2} \epsilon_0, \quad (2.9b)$$

$$Z_4 = -\frac{1}{8} \epsilon_0^2, \quad (2.9c)$$

⋮

and

$$\xi = \int^z Q(z) dz. \quad (2.10)$$

The  $(2N+1)$ th-order, or  $(N+1)$ -term, approximate solution of (2.4) is

$$q(z) = \sum_{j=0}^N q^{(2j+1)} = Q(z) \sum_{j=0}^N Y_{2j}. \quad (2.11)$$

Hereafter the simplest and most usual choice of  $Q(z)$  that generates the phase-integral approximation is used:  $Q^2(z) = R(z)$ . Then, from Eq. (2.5), the value of  $\epsilon_0$  is given by

$$\epsilon_0 = Q^{-3/2}(z) \frac{d^2}{dz^2} Q^{-1/2}(z). \quad (2.12)$$

At this point, some comments about the notation may be appropriate. In the present paper, the recent notation of Fröman and Fröman [10] is used,  $Q(z)$  and  $R(z)$  being the functions  $Q_{\text{mod}}(z)$  and  $Q(z)$ , respectively, of their previous papers [8,9,11,13–16].

The quantization condition of  $(2N+1)$ th order for a symmetric double-well potential obtained by Fröman *et al.* [15] reads

$$\alpha - \sigma \pm \frac{1}{2} \arctan[\exp(-\kappa)] = (n + \frac{1}{2})\pi, \quad n = 0, 1, 2, \dots, \quad (2.13)$$

where

$$\alpha = \sum_{j=0}^N \alpha^{(2j+1)}, \quad (2.14a)$$

$$\kappa = \sum_{j=0}^N \kappa^{(2j+1)}, \quad (2.14b)$$

$$\sigma = \sum_{j=0}^N \sigma^{(2j+1)}, \quad (2.14c)$$

with

$$\begin{aligned} \alpha^{(2j+1)} &= \text{Re} \left[ \frac{1}{2} \int_{\Gamma_\alpha} q^{(2j+1)} dz \right] \\ &= \text{Re} \left[ \frac{1}{2} \int_{\Gamma_\alpha} Y_{2j} d\xi \right], \end{aligned} \quad (2.15a)$$

$$\begin{aligned} \kappa^{(2j+1)} &= \frac{1}{2} i \int_{\Gamma_\kappa} q^{(2j+1)} dz \\ &= \frac{1}{2} i \int_{\Gamma_\kappa} Y_{2j} d\xi. \end{aligned} \quad (2.15b)$$

The first three terms of  $\sigma$  are

$$\sigma^{(1)} = \frac{1}{2} \left\{ -\arg \left[ \Gamma \left[ \frac{1}{2} + i \frac{\kappa}{\pi} \right] \right] + \frac{\kappa}{\pi} \ln \left| \frac{\kappa^{(1)}}{\pi} \right| - \frac{\kappa^{(1)}}{\pi} \right\}, \quad (2.16a)$$

$$\sigma^{(3)} = \frac{1}{2} \left[ 24 \frac{\kappa^{(1)}}{\pi} \right]^{-1}, \quad (2.16b)$$

$$\begin{aligned} \sigma^{(5)} &= \frac{1}{2} \left[ \frac{7}{2880} \left[ \frac{\kappa^{(1)}}{\pi} \right]^{-3} - \frac{1}{24} \frac{\kappa^{(3)}}{\pi} \left[ \frac{\kappa^{(1)}}{\pi} \right]^{-2} \right. \\ &\quad \left. + \frac{1}{2} \left[ \frac{\kappa^{(3)}}{\pi} \right]^2 \left[ \frac{\kappa^{(1)}}{\pi} \right]^{-1} \right]. \end{aligned} \quad (2.16c)$$

For energies far from the top of the intermediate barrier,  $\sigma$  can be neglected in the quantization condition (2.13), but close to the top of the barrier,  $\sigma$  must be included. The plus sign in Eq. (2.13) corresponds to an eigenfunction with even parity and the minus sign to one with odd parity. The contours of integration  $\Gamma_\alpha$  and  $\Gamma_\kappa$  are closed paths in the complex  $z$  plane encircling the classical turning points in the manner shown in Figs. 1 and 2 (see also Ref. [15]). Notice that the sign of the right-hand member of (2.15a) is opposite to that given in Ref. [15] because we have chosen the opposite direction for the integration contour. It should make no difference to use  $\Gamma'_\alpha$  instead of  $\Gamma_\alpha$  in (2.15a) since the quartic double well is symmetric.

The mathematical structure of (2.8) has the general form  $Y_{2n} = Z_{2n} + dU_{2n}/d\xi$ , and therefore, if  $\Gamma_\alpha$  and  $\Gamma_\kappa$  are closed contours, Eqs. (2.15) may be written in an equivalent and simpler form as

$$\alpha^{(2j+1)} = \text{Re} \left[ \frac{1}{2} \int_{\Gamma_\alpha} Z_{2j} d\xi \right], \quad (2.17a)$$

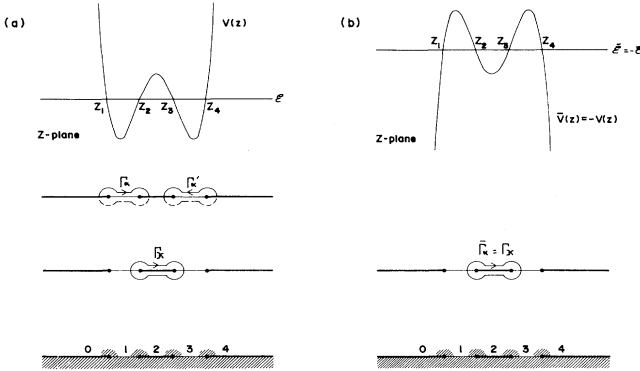


FIG. 1. (a) Quartic double-well potential showing the integration contours in the complex  $z$  plane in the sub-barrier case. The phase chosen is such that  $Q^{1/2}(z) = \exp[i(1-n)\pi/4]|Q(z)|^{1/2}$  on the real axis of the first Riemann sheet, where  $n$  is the region's index shown in the lower part of the figure. Cuts are shown by heavy lines. The parts of the contours that lie on the second Riemann sheet are indicated by dashed lines. (b) The quartic double well by means of the bar transformation:  $Q^{-1/2}(z) \rightarrow \bar{Q}^{-1/2}(z) = e^{i\pi/4}Q^{-1/2}(z)$ ,  $V(z) \rightarrow \bar{V}(z) = -V(z)$ ,  $\mathcal{E} \rightarrow \bar{\mathcal{E}} = -\mathcal{E}$ . The transformed integration contour  $\bar{\Gamma}_\alpha$  is shown. Here  $\bar{Q}^{-1/2}(z) = \exp[i(2-n)\pi/4]|Q(z)|^{1/2}$  on the real axis of the first Riemann sheet,  $n$  being the index of each region.

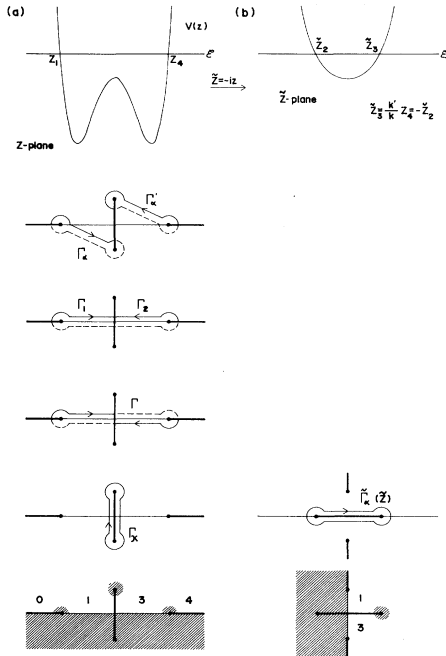


FIG. 2. (a) Quartic double-well potential showing the integration contours in the complex  $z$  plane in the superbarrier case. The phase chosen for  $Q^{1/2}(z)$  on the real axis of the first Riemann sheet is  $\exp[i(1-n)\pi/4]$ , where  $n$  is the index of each region. (b) The quartic single-well oscillator associated with the quartic double well by means of the tilde transformation:  $z \rightarrow \bar{z} = -iz$ ,  $Q^{1/2}(z) \rightarrow \bar{Q}^{1/2}(\bar{z}) = Q^{1/2}(z)$ ,  $V(z) = v_2z^2 + v_4z^4 \rightarrow \bar{V}(\bar{z}) = -v_2\bar{z}^2 + v_4\bar{z}^4$ ,  $\mathcal{E} \rightarrow \bar{\mathcal{E}} = \mathcal{E}$ . The transformed integration contour  $\bar{\Gamma}_\alpha(\bar{z})$  is shown. Here  $\bar{Q}^{1/2}(\bar{z}) = \exp[i(1-n)\pi/4]|Q(z)|^{1/2}$  on the real axis of the first Riemann sheet,  $n$  being the index of each region.

$$\kappa^{(2j+1)} = \frac{1}{2}i \int_{\Gamma_\kappa} Z_{2j} d\xi. \quad (2.17b)$$

In the next two sections we will show how to evaluate in terms of complete elliptic integrals all the integrals appearing in the quantization condition (2.13) for the sub-barrier and superbarrier cases.

### III. SUB-BARRIER CASE

The  $\alpha^{(2j+1)}$  integrals for the quartic double-well potential have already been calculated in Ref. [12]. For the sake of completeness we quote here the results up to fifth order. Let us define the function  $\mathcal{F}_j(\epsilon, w_2, w_4; \hat{K}, \hat{E})$  as

$$\mathcal{F}_j(\epsilon, w_2, w_4; \hat{K}, \hat{E}) = P_j(k^2) \frac{\hat{K} - \hat{E}}{k^2} + (-1)^j P_j(k'^2) \frac{\hat{E}}{k'^2}, \quad (3.1)$$

where

$$P_0(x) = \frac{\Omega k'^2}{6}, \quad (3.2a)$$

$$P_1(x) = \frac{k^2}{3\Omega} (1 + 4x), \quad (3.2b)$$

$$P_2(x) = -\frac{k^2}{45\Omega^3 k'^4} (56 - 153x + 285x^2 - 9320x^3 + 32400x^4 - 37632x^5 + 14336x^6), \quad (3.2c)$$

with

$$k^2 = \frac{\omega_4 A^2}{\omega_2 + 2\omega_4 A^2}, \quad (3.3a)$$

$$k'^2 = 1 - k^2, \quad (3.3b)$$

$$\Omega = [32\mu(\omega_2 + 2\omega_4 A^2)/\hbar^2]^{1/2} A^2. \quad (3.3c)$$

The quantity  $A$  is the amplitude of classical oscillations with energy  $\epsilon$  in the potential  $V(z) = w_2 z^4 + w_4 z^4$ , i.e., the energy and amplitude are related by

$$\epsilon = V(A) = w_2 A^2 + w_4 A^4. \quad (3.4)$$

In terms of the function  $\mathcal{F}_j$ , the  $\alpha^{(2j+1)}$  integrals [see Fig. 1(a)] with negative energy ( $\mathcal{E} < 0$ , sub-barrier case) are [12]

$$\alpha^{(2j+1)} = \mathcal{F}_j(\mathcal{E}, v_2, v_4; \frac{1}{2}\eta K(\eta^2), \frac{1}{2}\eta[E(\eta^2) - \eta'^2 K(\eta^2)]), \quad (3.5)$$

where the functions  $K$  and  $E$  are the complete elliptic integrals of the first and second kind, respectively [17]. The elliptic modulus is in this case  $\eta = 1/k$ . The complementary elliptic modulus is defined as  $\eta'^2 = 1 - \eta^2$ .

In order to evaluate the integrals appearing in the  $\kappa^{(2j+1)}$  terms [see Eqs. (2.15)], let us define

$$\bar{Q}^{1/2}(z) \equiv e^{i\pi/4} Q^{1/2}(z), \quad (3.6a)$$

$$\bar{\mathcal{E}} \equiv -\mathcal{E}, \quad (3.6b)$$

$$\bar{V}(z) \equiv \bar{v}_2 z^2 + \bar{v}_4 z^4 \equiv -V(z) = -v_2 z^2 - v_4 z^4. \quad (3.6c)$$

From these definitions, one concludes that

$$\bar{R}(z) \equiv \bar{Q}^2(z) \equiv \frac{2\mu}{\hbar^2} [\bar{\mathcal{E}} - \bar{V}(z)] = -Q^2(z). \quad (3.7)$$

Notice that in terms of barred quantities, the quartic double-well potential  $V(z)$  becomes a quartic double-barrier potential  $\bar{V}(z)$ , since  $\bar{v}_2 > 0$  and  $\bar{v}_4 < 0$  [see Fig. 1(b)]. Also we define

$$\bar{Z}_{2j} \equiv Z_{2j}(Q \rightarrow \bar{Q}) \equiv Z_{2j}(\bar{Q}), \quad (3.8a)$$

where the arrow means that  $Q(z)$  is replaced by  $\bar{Q}(z)$ , i.e.,  $\bar{Z}_{2j}(\bar{Q})$  are the expressions defined by Eqs. (2.9) with  $\epsilon_0$  given by Eq. (2.12) in which  $Q$  is replaced by  $\bar{Q}$ . Defining

$$d\bar{\xi} \equiv \bar{Q} dz, \quad (3.8b)$$

one obtains (see Appendix A)

$$Z_{2j} d\xi = (-1)^{j+1} i \bar{Z}_{2j} d\bar{\xi}, \quad (3.9)$$

and therefore Eq. (2.17b) becomes

$$\begin{aligned} \kappa^{(2j+1)} &= (-1)^j \frac{1}{2} \int_{\Gamma_\kappa} \bar{Z}_{2j} d\bar{\xi} \\ &= (-1)^j \frac{1}{2} \int_{\Gamma_\kappa} Z_{2j}(\bar{Q}) \bar{Q} dz. \end{aligned} \quad (3.10)$$

But, from Eq. (2.17a), the  $\alpha^{(2j+1)}$  term of the quartic double barrier  $\bar{V}(z)$ ,  $\alpha_{\text{DB}}^{(2j+1)}(\bar{\mathcal{E}}, \bar{v}_2, \bar{v}_4)$ , is given by

$$\alpha_{\text{DB}}^{(2j+1)}(\bar{\mathcal{E}}, \bar{v}_2, \bar{v}_4) = \text{Re} \left[ \frac{1}{2} \int_{\bar{\Gamma}_\alpha} \bar{Z}_{2j} d\bar{\xi} \right]. \quad (3.11)$$

Therefore, as  $\bar{\Gamma}_\alpha = \Gamma_\kappa$  and the integral of Eq. (3.11) is real (so that, actually, Re is not needed in this case), one finds, comparing Eq. (3.11) with Eq. (3.10), that

$$\begin{aligned} \kappa^{(2j+1)} &= (-1)^j \alpha_{\text{DB}}^{(2j+1)}(\bar{\mathcal{E}}, \bar{v}_2, \bar{v}_4) \\ &= (-1)^j \alpha_{\text{DB}}^{(2j+1)}(-\mathcal{E}, -v_2, -v_4). \end{aligned} \quad (3.12)$$

Explicit expressions for the terms  $\alpha_{\text{DB}}^{(2j+1)}$  are known [12]: using the function  $\mathcal{F}_j$  defined by Eqs. (3.1)–(3.4), the  $\kappa^{(2j+1)}$  term reads

$$\kappa^{(2j+1)} = (-1)^j \mathcal{F}_j \left[ \bar{\mathcal{E}}, \bar{v}_2, \bar{v}_4; \rho' K(\rho^2), \frac{E(\rho^2)}{\rho'} \right], \quad (3.13)$$

where

$$\rho^2 = -\frac{k^2}{1-k^2}, \quad (3.14a)$$

and

$$\rho'^2 = 1 - \rho^2. \quad (3.14b)$$

#### IV. SUPERBARRIER CASE

In the superbarrier case

$$\alpha^{(2j+1)} = \text{Re} \left[ \frac{1}{2} \int_{\Gamma_\alpha} Z_{2j} d\xi \right], \quad (4.1)$$

$\Gamma_\alpha$  being the integration contour shown in Fig. 2(a). This integral can be expressed equivalently as

$$\alpha^{(2j+1)} = \text{Re} \left[ \frac{1}{2} \int_{\Gamma_1} Z_{2j} d\xi \right], \quad (4.2)$$

where  $\Gamma_1$  is the open integration contour shown in Fig. 2(a). By the symmetry of the potential, we can write (4.2) as

$$\alpha^{(2j+1)} = \frac{1}{2} \text{Re} \left[ \frac{1}{2} \int_{\Gamma} Z_{2j} d\xi \right], \quad (4.3)$$

where  $\Gamma$  is the closed integration contour shown in Fig. 2(a). The integral of (4.3) has already been calculated in Ref. [12]. The result, in terms of the function  $\mathcal{F}_j$  defined through Eqs. (3.1)–(3.4), is

$$\alpha^{(2j+1)} = \frac{1}{2} \mathcal{F}_j(\mathcal{E}, v_2, v_4; K(k^2), E(k^2)). \quad (4.4)$$

Next we have to calculate the  $\kappa^{(2j+1)}$  integrals:

$$\kappa^{(2j+1)} = \frac{1}{2} i \int_{\Gamma_\kappa} Z_{2j} d\xi, \quad (4.5)$$

where now  $\Gamma_\kappa$  is an integration contour that encircles the imaginary turning points and the Stokes line [see Fig. 2(a)]. To evaluate these integrals we use the change of variable

$$\bar{z} \equiv -iz \quad (4.6)$$

and define

$$\bar{Q}^{1/2}(\bar{z}) \equiv Q^{1/2}(i\bar{z}) = Q^{1/2}(z). \quad (4.7)$$

Then

$$\begin{aligned} \bar{R}(\bar{z}) \equiv \bar{Q}^2(\bar{z}) &= Q^2(i\bar{z}) = \frac{2\mu}{\hbar^2} [\mathcal{E} - V(i\bar{z})] \\ &= \frac{2\mu}{\hbar^2} [\mathcal{E} - \bar{V}(\bar{z})], \end{aligned} \quad (4.8)$$

where the potential  $\bar{V}$  associated with  $V$  is given by

$$\bar{V}(\bar{z}) \equiv V(i\bar{z}) = -v_2 \bar{z}^2 + v_4 \bar{z}^4 \equiv \bar{v}_2 \bar{z}^2 + \bar{v}_4 \bar{z}^4. \quad (4.9)$$

Notice that  $\bar{V}(\bar{z})$  is, in terms of  $\bar{z}$ , a quartic single-well potential because  $\bar{v}_2 > 0$  and  $\bar{v}_4 > 0$ . With this transformation, the contour of integration  $\Gamma_\kappa$  is transformed into that termed  $\bar{\Gamma}_\alpha$  in Fig. 2(b). Next we define

$$\bar{Z}_{2j}(\bar{z}) \equiv Z_{2j}(Q \rightarrow \bar{Q}, z \rightarrow \bar{z}) \equiv Z_{2j}(Q^{1/2}(i\bar{z})), \quad (4.10)$$

i.e.,  $\bar{Z}_{2j}$  are the expressions defined by Eqs. (2.9),  $\epsilon_0$  being given by Eq. (2.12), but with  $Q$  and  $z$  replaced by  $\bar{Q}$  and  $\bar{z}$ , respectively. Defining

$$d\bar{\xi} = \bar{Q}(\bar{z}) d\bar{z}, \quad (4.11)$$

one obtains (see Appendix B)

$$\begin{aligned} Z_{2j}(z) d\xi &= (-1)^j i \bar{Z}_{2j}(\bar{z}) d\bar{\xi} \\ &= (-1)^j i \bar{Z}_{2j} \bar{Q} d\bar{z} \end{aligned} \quad (4.12)$$

and then  $\kappa^{(2j+1)}$  can be written in equivalent form as

TABLE I. Eigenvalues of the double-well quartic oscillator  $V(z) = -z^2 + 0.02z^4$  ( $W = \frac{25}{2}$ ) calculated using the phase-integral method of one, two, and three terms. Quoted values are the results of calculations shifted so as to make the minimum of the potential zero. In other words, the listed values  $E_n$  are defined as  $E_n = \mathcal{E}_n - V_{\min}$ . The upper (lower) value of each pair of eigenvalues corresponds to  $\sigma \neq 0$  ( $\sigma = 0$ ). Results obtained by Banerjee and Bhatnagar [6] are given for comparison. In this and the following tables the values are in units of  $\hbar^2/2\mu = 1$ . When  $E_n < W$ , that is, when  $\mathcal{E}_n < 0$ , the energy level lies below the top of the intermediate potential barrier, so that in this table all energy levels lie below the top of the barrier.

No. of terms	1	2	3	Banerjee and Bhatnagar
$E_0$	1.396 003 493	1.393 489 387	1.393 541 616	1.393 527 585
	1.398 900 695	1.393 535 083	1.393 352 764	
$E_1$	1.396 003 495	1.393 489 389	1.393 541 618	1.393 527 587
	1.398 900 697	1.393 535 085	1.393 527 643	
$E_2$	4.094 579 173	4.092 019 534	4.092 028 506	4.092 028 113
	4.098 402 813	4.092 043 891	4.092 028 337	
$E_3$	4.094 579 656	4.092 020 030	4.092 029 002	4.092 028 608
	4.098 403 299	4.092 044 387	4.092 028 832	

$$\begin{aligned} \kappa^{(2j+1)} &= (-1)^{j+1} \left[ \frac{1}{2} \int_{\tilde{\Gamma}_\alpha} \tilde{Z}_{2j} d\tilde{\xi} \right] \\ &= (-1)^{j+1} \left[ \frac{1}{2} \int_{\tilde{\Gamma}_\alpha} \tilde{Z}_{2j} \tilde{Q} d\tilde{z} \right]. \end{aligned} \tag{4.13}$$

But the expression in large parentheses is, by definition, the  $\alpha^{(2j+1)}$  integral of the single-well quartic potential  $\tilde{V}(\tilde{z})$ ,  $\alpha_{\text{SW}}^{(2j+1)}(\tilde{v}_2, \tilde{v}_4, \mathcal{E})$ , whose value (a real quantity) was obtained by Lakshmanan, Karlsson, and Fröman [11]. The result, in terms of the function  $\mathcal{F}_j$ , reads

$$\begin{aligned} \kappa^{(2j+1)} &= (-1)^{j+1} \alpha_{\text{SW}}^{(2j+1)}(\mathcal{E}, \tilde{v}_2, \tilde{v}_4) \\ &= (-1)^{j+1} \mathcal{F}_j(\mathcal{E}, \tilde{v}_2, \tilde{v}_4; K(k^2), E(k^2)). \end{aligned} \tag{4.14}$$

V. DISCUSSION OF RESULTS

In the preceding sections we have seen that the quantization condition for the quartic double well is given by

Eqs. (2.13)–(2.16), where, for the sub-barrier case, the term  $\alpha^{(2j+1)}$  is given by Eq. (3.5) and the  $\kappa^{(2j+1)}$  term is given by Eq. (3.13), and, for the superbarrier case, by Eqs. (4.4) and (4.14), respectively.

Some results for the energy levels of four different quartic double wells are listed in Tables I–IV. They are given in units of  $\hbar^2/2\mu = 1$  and taking as zero the bottom of the potential, that is, the listed energy is defined as  $E = \mathcal{E} - V_{\min}$ , where  $V_{\min} = -v_2^2/4v_4$ . The energy of the top of the internal barrier,  $W$ , is then equal to the difference between the potential maximum  $V_{\max} = 0$  and minimum  $V_{\min}$ , i.e.,  $W = V_{\max} - V_{\min} = -V_{\min}$ . Results are obtained using one, two, or three terms in the quantization conditions, and either including or neglecting  $\sigma$  in the calculations. The results are compared with those obtained by Banerjee and Bhatnagar [6] using a nonperturbative method of high accuracy. All the figures of the eigenenergies taken from this reference must be taken as exact. On the other hand, notice that the levels  $E_0$  and  $E_1$  lie close together and that, at some distance from

TABLE II. The same as Table I but now for the double-well oscillator  $V(z) = -z^2 + 0.05z^4$  ( $W = 5$ ). The upper (lower) value of each pair of eigenvalues corresponds to  $\sigma \neq 0$  ( $\sigma = 0$ ). Notice that all energy levels lie below the top of the intermediate potential barrier.

No. of terms	1	2	3	Banerjee and Bhatnagar
$E_0$	1.364 836 064	1.358 240 507	1.358 496 052	1.358 422 104
	1.373 813 656	1.358 625 895	1.358 448 198	
$E_1$	1.366 642 912	1.359 972 194	1.360 191 906	1.360 133 598
	1.375 439 241	1.360 358 883	1.360 144 188	
$E_2$	3.755 744 103	3.746 810 818	3.746 926 820	3.746 917 081
	3.780 025 943	3.750 441 457	3.747 717 326	
$E_3$	3.855 390 310	3.848 801 283	3.848 839 097	3.848 838 300
	3.886 782 620	3.853 572 993	3.848 585 280	

TABLE III. The same as Table I but now for the double-well oscillator  $V(z) = -z^2 + 0.07z^4$  ( $W = \frac{25}{7}$ ). The upper (lower) of each pair of eigenvalues corresponds to  $\sigma \neq 0$  ( $\sigma = 0$ ). Notice that only energy levels with  $E_n < W = \frac{25}{7} \approx 3.57$  lie below the intermediate potential barrier.

No. of terms	1	2	3	Banerjee and Bhatnagar
$E_0$	1.333 154 781	1.322 815 514	1.323 513 649	1.323 374 074
	1.347 888 175	1.324 152 994	1.323 595 043	
$E_1$	1.351 885 911	1.343 150 963	1.343 413 059	1.343 365 616
	1.367 291 489	1.344 562 268	1.343 512 492	
$E_2$	3.356 835 777	3.341 944 288	3.342 248 186	3.342 216 720
	3.389 316 732	3.301 967 381	3.214 441 023	
$E_3$	3.839 976 781	3.833 138 199	3.833 122 064	3.833 129 938
	3.785 338 131	3.485 417 279	3.973 632 973	

these levels, we have the levels  $E_2$  and  $E_3$ , which also lie close together (except in the neighborhood of and above the top of the barrier, i.e., for energy levels close to  $W$ ). This is indicated in Tables I–III by the use of brackets. Finally, in Table V we give this splitting of the energy levels for eigenvalues lying below the maximum of the intermediate barrier both with and without considering  $\sigma$  in the calculations.

From these tables some interesting conclusions may be drawn. For the double well with  $v_2 = -1$  and  $v_4 = 0.02$  (Table I), results obtained neglecting  $\sigma$  (i.e., taking  $\sigma = 0$ ) are very good: with the three-term approximation one obtains (except for the first level) at least seven significant figures in agreement. The results with  $\sigma \neq 0$  do not quite reach this level of agreement, although they are indeed still good: with three terms one achieves at least five significant figures of precision. All the eigenvalues are far from the critical zone, which is close to the top of the intermediate potential barrier ( $W = \frac{25}{2}$ ).

For the double well with  $v_2 = -1$  and  $v_4 = 0.05$  (Table II), results obtained with  $\sigma \neq 0$  are good (at least five accurate figures with the three-term approximation), including values near the critical zone. Results with  $\sigma = 0$

are also good except for energy levels close to the critical zone. From the other two cases,  $v_2 = -1$  with  $v_4 = 0.07$  (Table III) and  $v_2 = -1$  with  $v_4 = 0.15$  (Table IV), one reaches the same conclusion: for levels close to the top of the intermediate barrier the use of the simple value  $\sigma = 0$  is not good (i.e.,  $\sigma$  is not negligible), and results are very much better using the value of  $\sigma$  obtained from Eqs. (2.16). One can verify this assertion by comparing the precision of the values of  $E_2$  in Table III, or the values of  $E_0$  and  $E_1$  in Table IV, when  $\sigma$  is neglected ( $\sigma = 0$ ) and when the value of  $\sigma$  deduced from Eqs. (2.16) is used ( $\sigma \neq 0$ ). Fröman *et al.* [15] reached the same conclusion when analyzing a different double well (a harmonic well with an intermediate Gaussian barrier).

In Table V one can see that the values obtained for the splitting of the energy levels are excellent. Also one notices that, using the values of  $\sigma$  calculated with Eqs. (2.16), one obtains, in general, better results than using  $\sigma = 0$ . As expected, this is especially true for levels near the critical zone: see, for example, the values of  $\Delta_{01}$  for  $v_4 = 0.15$  or the values of  $\Delta_{23}$  for  $v_4 = 0.05$ . As observed in the discussion of Fröman (Ref. [13], p. 92), the energy splittings are obtained with a greater absolute accuracy

TABLE IV. The same as Table I but now for the double-well oscillator  $V(z) = -z^2 + 0.15z^4$  ( $W = \frac{5}{3}$ ). The upper (lower) of each pair of eigenvalues corresponds to  $\sigma \neq 0$  ( $\sigma = 0$ ). Notice that only energy levels with  $E_n < W = \frac{5}{3} \approx 1.67$  lie below the intermediate potential barrier.

No. of terms	1	2	3	Banerjee and Bhatnagar
$E_0$	1.092 241 166	1.058 655 332	1.065 780 880	1.062 499 248
	1.133 492 490	1.061 913 628	1.041 856 344	
$E_1$	1.430 778 772	1.421 818 391	1.420 241 606	1.421 086 891
	1.490 548 207	1.762 589 357	1.937 765 226	
$E_2$	3.043 422 995	3.033 869 600	3.033 585 921	3.033 667 277
	3.011 284 522	3.030 496 428	3.033 516 677	
$E_3$	4.591 591 012	4.590 094 588	4.589 809 057	4.589 838 496
	4.572 393 252	4.589 447 462	4.589 653 663	

TABLE V. Energy splittings in the sub-barrier case,  $E_1 - E_0 \equiv \Delta_{01}$  and  $E_3 - E_2 \equiv \Delta_{23}$ , calculated with the three-term (fifth-order) phase-integral approximation, compared with the values given by Banerjee and Bhatnagar [6] for the double wells  $V(z) = -z^2 + v_4 z^4$  considered in Tables I–IV. Notice that for  $V(z) = -z^2 + 0.15z^4$  and  $\sigma = 0$ , the eigenvalue  $E_1$  lies above the top of the barrier in the approximation considered (see Table IV).

$v_4$	$\Delta_{ij}$	$\sigma \neq 0$	$\sigma = 0$	Banerjee and Bhatnagar
0.02	$\Delta_{01}$	0.000 000 002	0.000 174 879	0.000 000 002
	$\Delta_{23}$	0.000 000 496	0.000 000 495	0.000 000 495
0.05	$\Delta_{01}$	0.001 695 854	0.001 695 990	0.001 711 494
	$\Delta_{23}$	0.101 912 277	0.100 867 954	0.101 921 219
0.07	$\Delta_{01}$	0.019 899 410	0.019 917 449	0.019 991 542
0.15	$\Delta_{01}$	0.354 460 726	0.895 908 882	0.358 587 643

than the eigenenergies themselves. This phenomenon is most notable for levels that lie far below the barrier maximum.

Finally, one must notice that Eqs. (2.16) were derived under the assumption that the transition zeros associated with the barrier lie sufficiently far away from all other transition zeros. If this is not the case, it sometimes happens (especially if the energy lies far away from the top of the barrier) that one obtains an energy level more accurately when  $\sigma$  is neglected than when  $\sigma$  is calculated according to Eqs. (2.16).

## VI. CONCLUDING REMARKS

The integrals appearing in the quantization conditions of the phase-integral method of Fröman and Fröman up to fifth order have been explicitly obtained for the double-well quartic oscillator. The terms  $\alpha^{(2j+1)}$  and  $\kappa^{(2j+1)}$  appearing in the quantization condition, Eq. (2.13), are given by Eqs. (3.5) and (3.13), respectively, for the sub-barrier case, and by Eqs. (4.4) and (4.14), respectively, for the superbarrier case. For both cases the  $\alpha^{(2j+1)}$  terms have already been calculated in Ref. [12]. To evaluate the  $\kappa^{(2j+1)}$  terms, we have used an indirect method. For both cases (sub-barrier and superbarrier), we have shown that each  $\kappa^{(2j+1)}$  term is proportional to the  $\alpha^{(2j+1)}$  term of an associated quartic oscillator:  $\kappa^{(2j+1)} = c_j \alpha_{\text{assoc}}^{(2j+1)}$ . For the sub-barrier case, the quartic oscillator associated with the quartic double well  $V(z) = v_2 z^2 + v_4 z^4$  ( $v_2 < 0$  and  $v_4 > 0$ ) with energy  $\mathcal{E}$  is the quartic double barrier  $V(z) = -v_2 z^2 - v_4 z^4$  with energy  $-\mathcal{E}$  and  $c_j = (-1)^j$ . For the superbarrier case, the quartic oscillator associated with the quartic double well  $V(z) = v_2 z^2 + v_4 z^4$  ( $v_2 < 0$  and  $v_4 > 0$ ) with energy  $\mathcal{E}$  is the quartic single well  $V(z) = -v_2 z^2 + v_4 z^4$  with the same energy  $\mathcal{E}$  and  $c_j = (-1)^{j+1}$ . The key point is that the  $\alpha^{(2j+1)}$  terms of the associated oscillator have already been calculated for the single well in Ref. [11], and for

the quartic double barrier in Ref. [12]. Using these expressions in the phase-integral quantization condition of order  $2N + 1$  ( $N = 0, 1, 2$ ), accurate values have been obtained for the eigenenergies in both the sub-barrier and superbarrier region, including the intermediate or critical zone close to the top of the barrier.

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## APPENDIX A

In this appendix we prove Eq. (3.9). From the definitions of Eqs. (3.6) one has that

$$Q = c\bar{Q}, \quad c = -i, \quad (\text{A1})$$

and from Eqs. (2.10) and (3.8) one finds

$$d\xi = Q dz = c\bar{Q} dz = c d\bar{\xi}. \quad (\text{A2})$$

Applying the change  $Q \rightarrow \bar{Q}$  to Eq. (2.12), the quantity  $\epsilon_0$  is converted to

$$\epsilon_0 = \bar{Q}^{-3/2}(z) \frac{d^2}{dz^2} \bar{Q}^{-1/2}(z). \quad (\text{A3})$$

From (A1) it is easy to see that  $\bar{\epsilon}_0 = c^2 \epsilon_0$ . Therefore, from Eqs. (2.9), one finds

$$\begin{aligned} \bar{Z}_0 &= 1 = Z_0, \\ \bar{Z}_2 &= \frac{1}{2} \bar{\epsilon}_0 = c^2 Z_2, \\ \bar{Z}_4 &= -\frac{1}{8} \bar{\epsilon}_0^2 = c^4 Z_4. \end{aligned} \quad (\text{A4})$$

Using Eqs. (A2) and (A4) and substituting the value of  $c$ , Eq. (A1), one proves that  $Z_{2j} d\xi$  is given by Eq. (3.9).

## APPENDIX B

In this appendix we prove Eq. (4.12). Taking into consideration (2.10) and (4.11), one easily finds that

$$d\xi = i d\tilde{\xi}. \quad (\text{B1})$$

Applying the changes  $Q \rightarrow \tilde{Q}$  and  $z \rightarrow \tilde{z}$  to Eq. (2.12), the quantity  $\epsilon_0$  is converted to

$$\tilde{\epsilon}_0 = \tilde{Q}^{-3/2}(\tilde{z}) \frac{d^2}{d\tilde{z}^2} \tilde{Q}^{-1/2}(\tilde{z}). \quad (\text{B2})$$

From Eqs. (4.6) and (4.7) one easily finds that  $\tilde{\epsilon}_0 = -\epsilon_0$ . Then, from Eqs. (2.9) one has

$$\begin{aligned} \tilde{Z}_0 &= 1 = Z_0, \\ \tilde{Z}_2 &= \frac{1}{2} \tilde{\epsilon}_0 = -Z_2, \\ \tilde{Z}_4 &= -\frac{1}{8} \tilde{\epsilon}_0^2 = Z_4. \end{aligned} \quad (\text{B3})$$

From Eqs. (B1) and (B3), one deduces Eq. (4.12).

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