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PHASE-INTEGRAL APPROACH TO ROSEN-MORSE POTENTIALS

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We apply the phase-integral condition to the motion of a quantal particle in the Rosen-Morse potential $V(x) = B_0 \tanh(x/x_0) - U_0 \cosh^{-2}(x/x_0)$ to show that it yields the energy eigenvalues exactly in any order of approximation, when the base function is chosen conveniently. Thereafter, we show that the phase-integral formula for the normalization factors of bound states agrees very satisfactorily with the exact calculation. Finally, we apply the phase-integral formula for the reflexion coefficient to the transmission of a quantal particle through the above potential to show that it gives very accurate results.

1. *Introduction*

The calculation of the exact bound-state energy eigenvalues, the normalization factors and reflexion coefficients for a quantal particle in the Rosen-Morse potential

$$V(x) = B_0 \tanh(x/x_0) - U_0 \cosh^{-2}(x/x_0) \tag{1.1}$$

has been performed in Refs. 1, 2 and 3, respectively. The investigation of the potential (1.1) started in early days of the development of quantum mechanics when it was used as a model potential in the study of the vibrations of certain polyatomic molecules along a given axis. During the further development of quantum mechanics this potential has also been used for other purposes. The symmetric form of the potential (1.1) obtained when $B_0 = 0$, occurs for example in the study of solitons. An extensive list of references on particular applications of the potential (1.1) is found in Ref. 2.

The aim of the present paper is to investigate the application of the phase-integral method (i.e. the improved JWKB method) to the motion of a quantal particle in the potential (1.1). We consider the bound-state energy eigenvalues, normalization factors of bound states and reflexion coefficients and compare the phase-integral results with the exact results given in Refs. 1–3. Although these exact results are known, the application of the phase-integral method to this potential is of interest to show the power of the phase-integral method and the high accuracy of the results.

The time-independent Schrödinger equation for the motion of a quantal particle, with energy E and mass M, in the one-dimensional potential (1.1), can be written as

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}z^2} + R(z)\Psi = 0, \tag{1.2}$$

where $z = x/x_0$ is the dimensionless variable and

$$R(z) = A - B\tanh z - C\tanh^2 z \tag{1.3}$$

is the dimensionless function.

In Eq. (1.3) we introduced

$$A = \frac{2Mx_0^2}{\hbar^2}(E + U_0) \tag{1.4a}$$

$$B = \frac{2Mx_0^2}{\hbar^2}B_0 \tag{1.4b}$$

$$C = \frac{2Mx_0^2}{\hbar^2}U_0 \tag{1.4c}$$

and the bound-states in the potential (1.1) may exist if the conditions

$$C > 0 \tag{1.5a}$$

$$|B| < 2C \tag{1.5b}$$

$$-\frac{B^2}{4C} < A < C - |B| \tag{1.5c}$$

are satisfied.

2. Review of the exact results

2.1. Bound states

2.1.1. Bound-state energy eigenvalues

The problem of finding the bound states in the potential (1.1) has been considered in Ref. 1 and in our notation the exact bound-state energies, obtained from (6c) in Ref. 1, are

$$E_S = -\frac{\hbar^2}{2Mx_0^2}(m-s)^2 - \frac{2Mx_0^2}{\hbar^2}\frac{B_0^2}{4(m-s)^2}, \tag{2.1}$$

where s is an integer satisfying inequality

$$0 < s < m - \left(\frac{|B|}{2}\right)^{1/2}, \tag{2.2}$$

and m is a positive real number (cf. Eq. (3.6) in Ref. 2)

$$m = (C + \frac{1}{4})^{1/2} - \frac{1}{2}. \tag{2.3}$$

Using (1.4a,b,c) Eq. (2.1) gives

$$A - C = -(m-s)^2 - \frac{B^2}{4(m-s)^2}. \tag{2.4}$$

Solving Eq. (2.4) for $(m-s)$, with due regard to (2.2) and (2.3), gives the exact quantization condition

$$(C + \frac{1}{4})^{1/2} - \frac{1}{2}(C - A + B)^{1/2} - \frac{1}{2}(C - A - B)^{1/2} = s + \frac{1}{2}. \tag{2.5}$$

2.1.2. Bound state wave functions

The exact normalized bound-state wave functions corresponding to the energy eigenvalues (2.1) are given by Eq. (3.5) in Ref. 2, which in our notation reads

$$\Psi_S = N_{RM}(s) e^{pz} \cosh^{-m+s} z F(-s, 2m-s+1; m-s+p+1; u) \tag{2.6}$$

where (cf. Eq. (3.7) in Ref. 2, where U_0 should be replaced by B_0 and a missing sign should be introduced)

$$p = -\frac{B}{2(m-s)}, \quad u = \frac{1}{2}(1+\tanh z) \tag{2.7}$$

and $N_{RM}(s)$ is given by Eq. (3.15) in Ref. 2, which in our notation reads

$$N_{RM}(s) = (2\pi x_0)^{-1/2}$$

$$\cdot \left(\frac{2\pi\Gamma(m-\frac{s}{2}+\frac{1}{2})\Gamma(m-\frac{s}{2}+1)\Gamma(m-s-p+1)\Gamma(m+p+1)}{(m-s)\Gamma(\frac{s}{2}+\frac{1}{2})\Gamma(\frac{s}{2}+1)\Gamma(m-s+p)\Gamma(m-s-p)\Gamma(m-s+p+1)\Gamma(m-p+1)} \right)^{1/2}. \tag{2.8}$$

2.1.3. Asymptotic form of the wave function in the limit $z \to +\infty$

In the limit $z \to +\infty$ the exact wave function (2.6) acquires the following form

$$\Psi_S = G_e \exp\left[-(m-s-p)z\right] \tag{2.9}$$

where

$$G_e = 2^{m-s} N_{RM}(s) F(-s, 2m-s+1; m-s+p+1; 1). \tag{2.10}$$

Using (2.7) and the formulae

$$F(\alpha, \beta; \gamma; 1) = \frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)},$$

$$\gamma \neq 0, -1, -2, \dots, \quad \mathrm{Re}(\gamma-\alpha-\beta) \geq 0, \tag{2.11}$$

$$\Gamma(2z) = (2\pi)^{-1/2} 2^{2z-1/2} \Gamma(z)\Gamma(z+\frac{1}{2}), \tag{2.12}$$

$$\Gamma(z+1) = z\Gamma(z) \tag{2.13}$$

Eqs. (2.10) and (2.8) give the following result

$$G_e = (2\pi x_0)^{-1/2}\left(1+\frac{p}{m-s}\right)^{1/2}\frac{\sqrt{2\pi(m-s-p)}}{\Gamma(m-s-p+1)}$$

$$\cdot\left[\frac{\Gamma\left(2m-s+\frac{1}{2}+\frac{1}{2}\right)}{\Gamma\left(s+\frac{1}{2}+\frac{1}{2}\right)}\right]^{1/2}\left[\frac{\Gamma\left(m+\frac{1}{2}-p+\frac{1}{2}\right)}{\Gamma\left(m+\frac{1}{2}+p+\frac{1}{2}\right)}\right]^{1/2}. \tag{2.14}$$

Using the asymptotic formula for the gamma function given by Eq. (5) in Section 2.11 of Ref. 4, i.e.

$$\Gamma\left(z+\frac{1}{2}\right) = \sqrt{2\pi}\,(z/e)^z\exp\left(-\frac{1}{24z}+\frac{7}{2880z^3}-\frac{31}{40320z^5}+\,...\right),$$

$$|\arg\ z| < \pi-\epsilon,\quad \epsilon>0, \tag{2.15}$$

in the fourth and fifth factor of (2.14) and Stirling's formula, given by Eq. (1) in Section 2.11 of Ref. 4, i.e.

$$\Gamma\left(z+1\right) = \sqrt{2\pi z}\,(z/e)^z\exp\left(\frac{1}{12z}-\frac{1}{360z^3}+\frac{1}{1260z^5}-\,...\right),$$

$$|\arg\ z| < \pi-\epsilon,\quad \epsilon>0, \tag{2.16}$$

in the third factor of (2.14) gives

$$G_e = (2\pi x_0)^{-1/2}\left(1+\frac{p}{m-s}\right)^{1/2}$$

$$\cdot\frac{\left(2m-s+\frac{1}{2}\right)^{(1/2)(2m-s+1/2)}}{(m-s-p)^{(m-s-p)}\left(s+\frac{1}{2}\right)^{(1/2)(s+1/2)}}\left(\frac{m+\frac{1}{2}-p}{m+\frac{1}{2}+p}\right)^{(1/2)(m+1/2)}\left[\left(m+\frac{1}{2}\right)^2-p^2\right]^{-p/2}$$

$$\cdot\exp\left[\frac{1}{48}\left(\frac{1}{m+\frac{1}{2}+p}-\frac{1}{m+\frac{1}{2}-p}+\frac{1}{s+\frac{1}{2}}-\frac{1}{2m-s+\frac{1}{2}}-\frac{4}{m-s-p}\right)+\right.$$

$$\frac{1}{360}\left(-\frac{7}{16(m+\frac{1}{2}+p)^3}+\frac{7}{16(m+\frac{1}{2}-p)^3}-\frac{7}{16(s+\frac{1}{2})^3}+\right.$$

$$\left.+\frac{7}{16(2m-s+\frac{1}{2})^3}-\frac{1}{(m-s-p)^3}\right)+\dots\Bigg]. \tag{2.17}$$

2.2. The reflexion coefficient

The exact reflexion coefficient for the transmission of a quantal particle through the potential (1.1) is given by Eq. (15) in Ref. 3 and in our notation it can be written in the form

$$R_e=\frac{\cosh\left(\pi\sqrt{A+B-C}-\pi\sqrt{A-B-C}\right)+\cosh\left(2\pi\sqrt{-C-\frac{1}{4}}\right)}{\cosh\left(\pi\sqrt{A+B-C}+\pi\sqrt{A-B-C}\right)+\cosh\left(2\pi\sqrt{-C-\frac{1}{4}}\right)}. \tag{2.18}$$

3. Review of the phase-integral method

3.1. Bound states

3.1.1. Bound-state energy eigenvalues

The eigenvalue problem of finding the bound-state energies in the potential (1.1), when the conditions (1.5a,b,c) are fulfilled, is solved by means of the phase-integral quantization condition, which in the $(2N+1)$-th order approximation reads (c.f. Eq. (10.20) in Ref. 5 and Refs. 6–8)

$$\sum_{n=0}^{N}L^{(2n+1)}=\left(s+\frac{1}{2}\right)\pi,\quad s=0,1,2,\dots, \tag{3.1}$$

with

$$L^{(2n+1)}=\frac{1}{2}\int_{\Lambda}Z_{2n}Q(z)\,\mathrm{d}z, \tag{3.2}$$

where $Q(z)$ is a so far unspecified base function, and

$$Z_0=1\ ,\ Z_2=\epsilon_0/2\ ,\ Z_4=\epsilon_0^2/8,\ \dots \tag{3.3}$$

with

$$\epsilon_0 = Q^{-3/2}(z)\frac{\mathrm{d}^2}{\mathrm{d}z^2}Q^{-1/2}(z) + \frac{R(z) - Q^2(z)}{Q^2(z)}. \tag{3.4}$$

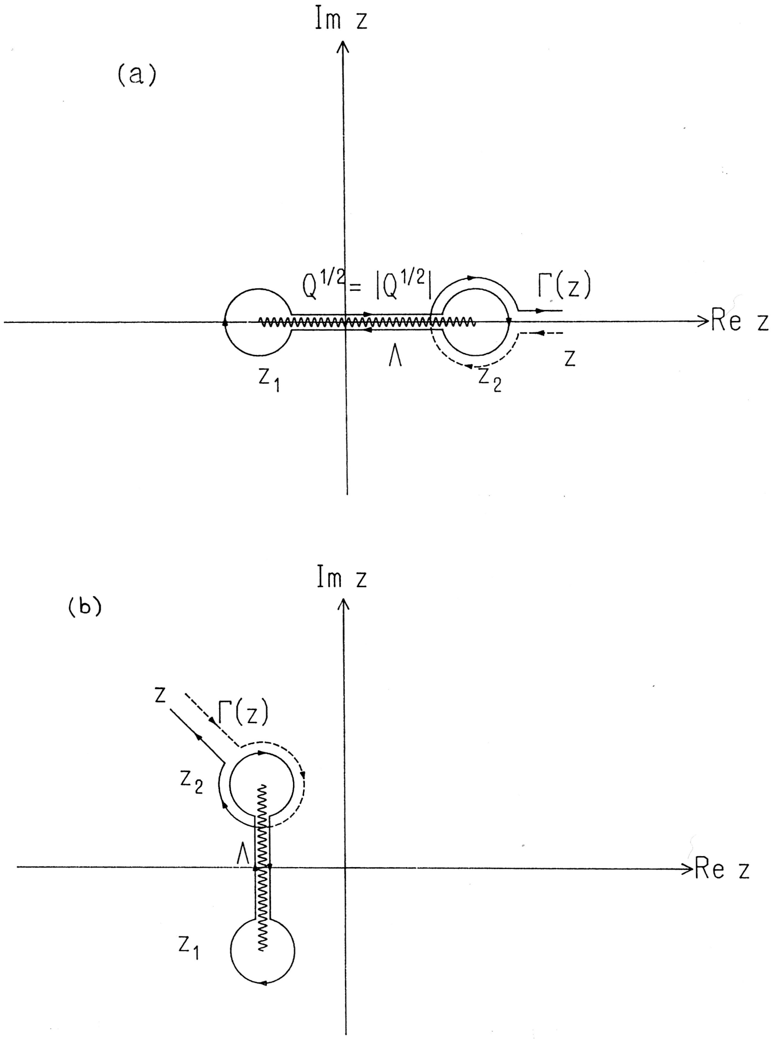

Fig. 1. The contours Λ and $\Gamma(z)$ in the complex z-plane with the phase of $Q^{1/2}(z)$: (a) Transition points are on the real axis; (b) Transition points are not on the real axis.

The contour Λ in (3.2) encircles in the clockwise sense the two zeroes of $Q^2(z)$, which are called generalized classical turning points or simply turning points. The contour Λ with the phase for $Q^{1/2}(z)$ and the corresponding branch cut in the z-plane is shown in Fig. 1a.

3.1.2. Bound-state wave functions and normalization factors

The phase-integral formula for the normalization factor of a bound-state wave function in a single-well potential is given in Refs. 9 and 10. The normalized phase-integral wave function, given by Eq. (30c) in Ref. 9, on the real axis to the right of the turning point z_2 in Fig. 1a, has in this region the form

$$\Psi(z) = N_{PI} q^{-1/2}(z) \exp\{-\mathrm{i}[w(z) - \pi/4]\}, \quad z > z_2 \tag{3.5}$$

where $q(z)$ is given by

$$q(z) = \sum_{n=0}^{N} q^{(2n+1)}(z) = \sum_{n=0}^{N} Y_{2n} Q(z) \tag{3.6}$$

with

$$Y_0 = 1\ , \quad Y_2 = \epsilon_0/2\ , \quad Y_4 = -\frac{\epsilon_0^2}{8} - \frac{1}{8}\frac{\mathrm{d}^2\epsilon_0}{\mathrm{d}\zeta^2}\ , \ \ldots \tag{3.7}$$

and

$$\zeta = \int^{z} Q(z)\mathrm{d}z \tag{3.8}$$

while $w(z)$ is given by

$$w(z) = \sum_{n=0}^{N} w^{(2n+1)}(z) \tag{3.9}$$

with

$$w^{(2n+1)}(z) = \frac{1}{2} \int_{\Gamma(z)} Y_{2n} Q(z)\,\mathrm{d}z, \tag{3.10}$$

and the contour $\Gamma(z)$ is shown in Fig. 1a.

The normalization factor N_{PI} in (3.5) is given by the approximate formula

$$|N_{PI}^2| = \frac{Mx_0}{2\pi\hbar^2}\frac{\mathrm{d}E_s}{\mathrm{d}s}, \tag{3.11}$$

where E_s is the energy of a bound state labeled by the quantum number s.

3.2. *The reflexion coefficient*

When the potential (1.1) has a shape of a barrier, the phase-integral formula for the reflexion coefficient, in the $(2n+1)$th-order, is given by (cf. Ref. 11)

$$R = \frac{1}{1+\exp(-2K)} \tag{3.12}$$

where

$$K = \sum_{n=0}^{N} K^{(2n+1)} \tag{3.13}$$

and $K^{(2n+1)}$ are real quantities defined by

$$K^{(2n+1)}(z) = \frac{\mathrm{i}}{2}\int_{\Lambda} Z_{2n}Q(z)\,\mathrm{d}z, \tag{3.14}$$

with the contour Λ shown in Fig. 1b.

4. *Phase-integral calculation*

In the present paper we choose the square of the base function $Q^2(z)$ in the form

$$Q^2(z) = a - b\tanh z - c\tanh^2 z, \tag{4.1}$$

where a, b and c are parameters to be chosen later.

4.1. *Bound states*

4.1.1. *Bound-state energy eigenvalues*

We now calculate the integrals (3.2) up to the fifth order approximation ($n = 0,\ 1,\ 2$) and show that when the parameters a, b and c are chosen in such a way that the higher-order contributions ($n = 1,\ 2$) vanish, the first-order phase-integral quantization condition (3.1) agrees with the exact quantization condition (2.5). To simplify the calculation we introduce the new variable

$$t = \tanh z. \tag{4.2}$$

Then (3.2) becomes

$$L^{(2n+1)} = \frac{1}{2} \int\limits_{\Lambda_t} Z_{2n} Q \frac{\mathrm{d}t}{1-t^2} \tag{4.3}$$

where Λ_t (See Fig. 2) is a contour in the complex t-plane which corresponds to the contour Λ in the complex z-plane. It encircles the zeroes of Q^2, which according to (4.1) and (4.2) are

$$t_{1,2} = -\frac{b}{2c} \pm \left[\frac{b^2}{4c^2} + \frac{a}{c} \right]^{1/2},$$

but it does not encircle the points $t = \pm 1$.

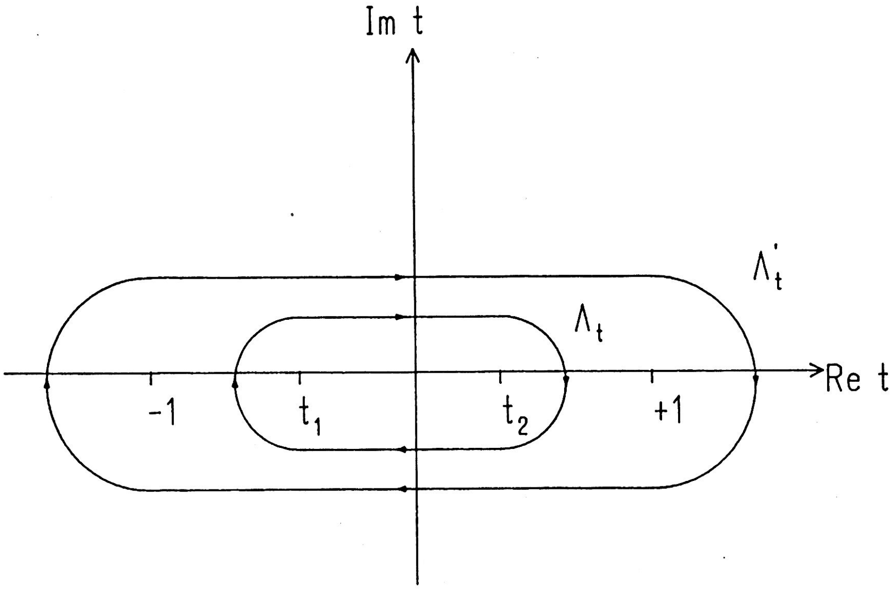

Fig. 2. The contours Λ_t and Λ_t' in the complex t-plane.

From (4.3) we obtain

$$L^{(2n+1)} = \frac{1}{2}\int\limits_{\Lambda_t'} Z_{2n}Q\frac{\mathrm{d}t}{1-t^2} + \pi\mathrm{i}\left(\operatorname*{Res}_{t=+1}\frac{Z_{2n}Q}{1-t^2} + \operatorname*{Res}_{t=+1}\frac{Z_{2n}Q}{1-t^2}\right) \tag{4.4}$$

where Λ_t' (see Fig.2) is a contour which encircles both the points t_1 and t_2 and the points $t = \pm 1$. Since there are no singular points of the integrand in (4.4) outside the contour Λ_t', it can be extended to infinity. Using Eqs. (3.3), (3.4), (4.1) and (4.2), we obtain

$$Q \to -\mathrm{i}\sqrt{c}t, \quad \text{as} \quad |t| \to \infty \tag{4.5}$$

$$Z_{2n} \to \delta_{n,0} + \frac{C+\frac{1}{4}-c}{2c}\delta_{n,1} - \frac{(C+\frac{1}{4}-c)^2}{8c^2}\delta_{n,2}$$

$$n = 0,\ 1,\ 2 \quad \text{as} \quad |t| \to \infty. \tag{4.6}$$

Performing now simple residue calculations, using (4.1), (4.2) and (4.6), we obtain

$$L^{(2n+1)} = \pi\sqrt{c}\delta_{n,0} + \pi\frac{C+\frac{1}{4}-c}{2\sqrt{c}}\delta_{n,1} - \pi\frac{(C+\frac{1}{4}-c)^2}{8c^{3/2}}\delta_{n,2} -$$

$$-\frac{\pi}{2}\sqrt{c-a+b}Z_{2n}(t=+1) - \frac{\pi}{2}\sqrt{c-a-b}Z_{2n}(t=-1), \quad n = 0,\ 1,\ 2. \tag{4.7}$$

Inserting (4.6) into (4.7) we obtain

$$L^{(1)} = \pi\left(\sqrt{c} - \frac{1}{2}\sqrt{c-a+b} - \frac{1}{2}\sqrt{c-a-b}\right), \tag{4.8a}$$

$$L^{(3)} = \pi\frac{C+\frac{1}{4}-c}{2\sqrt{c}} - \frac{\pi}{4}\left(\frac{D_+}{\sqrt{c-a+b}} + \frac{D_-}{\sqrt{c-a-b}}\right), \tag{4.8b}$$

$$L^{(5)} = -\pi\frac{(C+\frac{1}{4}-c)^2}{8c^{3/2}} + \frac{\pi}{16}\left(\frac{D_+^2}{\sqrt{(c-a+b)^3}} + \frac{D_-^2}{\sqrt{(c-a-b)^3}}\right) \tag{4.8c}$$

where $D_\pm = (C-c) - (A-a) \pm (B-b)$. We now choose the parameters a, b and c in such a way that all higher contributions ($n = 1,\ 2$) on the left hand side of the quantization condition (3.1) vanish, and that in any order of approximation the only surviving term is $L^{(1)}$. From (4.8a, b, c) we see that it is the case if

$$a = A + \frac{1}{4}, \quad b = B, \quad c = C + \frac{1}{4}. \tag{4.9}$$

Thus the phase-integral quantization condition (3.1) in any order of approximation becomes

$$\sqrt{c} - \frac{1}{2}\sqrt{c-a+b} - \frac{1}{2}\sqrt{c-a-b} = s + \frac{1}{2}, \quad s = 0,\ 1,\ 2,\ \ldots \tag{4.10}$$

and in view of (4.9) it is identical to the exact quantization condition (2.5). The square of the base function $Q^2(z)$ is then given by

$$Q^2(z) = R(z) + \frac{1}{4\cosh^2 z}. \tag{4.11}$$

4.1.2. Bound-state wave function and normalization factors

Inserting (2.1) into (3.11), we obtain

$$|N_{PI}^2| = \frac{1}{2\pi x_0}(m-s)\left[1 - \frac{p^2}{(m-s)^2}\right]. \tag{4.12}$$

Using (1.3), (3.4), (3.7), (4.1) and (4.2) we now calculate the integrals (3.10) to obtain

$$w^{(1)}(z) = -\frac{\mathrm{i}}{2}\left[\sqrt{c-a+b} + \sqrt{c-a-b}\right] z - \frac{\mathrm{i}}{2}\left[\sqrt{c-a+b} + \sqrt{c-a-b}\right]\ln(e^z + e^{-z}) +$$

$$+\mathrm{i}\sqrt{c-a-b}\ln\left[b+2a+(2c-b)\tanh z - 4\sqrt{c-a-b}\sqrt{c\tanh^2 z + b\tanh z - a}\right] -$$

$$-\mathrm{i}\sqrt{c-a+b}\ln\left[b-2a+(2c+b)\tanh z + 4\sqrt{c-a+b}\sqrt{c\tanh^2 z + b\tanh z - a}\right] +$$

$$+\frac{\mathrm{i}\sqrt{c}}{2}\ln\left[\frac{b}{2} + c\tanh z - \sqrt{c}\sqrt{c\tanh^2 z + b\tanh z - a}\right] -$$

$$-\frac{\mathrm{i}\sqrt{c}}{2}\ln\left[\frac{b}{2} + c\tanh z + \sqrt{c}\sqrt{c\tanh^2 z + b\tanh z - a}\right] +$$

$$+\frac{\mathrm{i}}{4}\left[\sqrt{c-a+b}-\sqrt{c-a-b}\right]\ln(ca+\frac{b^2}{4}) \tag{4.13a}$$

$$w^{(3)}(z)=-\frac{\mathrm{i}}{8}\frac{(2b^2+4ac)\tanh z-2ab}{(b^2+4ac)\sqrt{c\tanh^2 z+b\tanh z-a}}$$

$$\cdot\left[1-\frac{b^2+4ac}{12c[(b^2+2ac)\tanh z-ab]}\right.$$

$$\cdot\left(\frac{(2c\tanh z+b)(4c^2-4ac+b^2)}{b^2+4ac}-\frac{[b^2+2c(c-a)]\tanh z-b(a+c)}{c\tanh^2 z+b\tanh z-a}\right)-$$

$$\left.-\frac{(b^2+4ac)(2c\tanh z-b)(1-\tanh^2 z)}{2[(b^2+2ac)\tanh z-ab](c\tanh^2 z+b\tanh z-a)}\right] \tag{4.13b}$$

$$w^{(5)}(z)=-\frac{\mathrm{i}(2c\tanh z+b)}{192c^2(b^2+4ac)\sqrt{c\tanh^2 z+b\tanh z-a}}$$

$$\cdot\left\{12c^2-12ac+b^2+\frac{6c^4+28ac^3-18a^2c^2+28ab^2c-38b^2c^2+19b^4}{6c}\right.$$

$$\cdot\left(\frac{1}{c\tanh^2 z+b\tanh z-a}-\frac{8b}{b^2+4ac}\right)-\frac{1}{60c^2}\left(28c^6-36ac^5+20a^2c^4-\right.$$

$$\left.-12a^3c^3+82a^2b^2c^2+112ab^2c^3-62ab^4c-30b^2c^4+32b^4c^2-11b^6\right)$$

$$\cdot\left[\frac{3}{(c\tanh^2 z+b\tanh z-a)^2}-\frac{16c}{(b^2+4ac)(c\tanh^2 z+b\tanh z-a)}+\right.$$

$$\left.\left.+\ \frac{128c^2}{(b^2+4ac)^2}\right]\right\}+\frac{\mathrm{i}b}{128c^2\sqrt{c\tanh^2 z+b\tanh z-a}}$$

$$\cdot\left[1+\frac{6c^2+6ac-8b^2}{9c(c\tanh^2 z+b\tanh z-a)}-\right.$$

$$\left.-\frac{40c^4-48ac^3+24a^2c^2+40ab^2c-32b^2c^2+11b^4}{30c^2(c\tanh^2 z+b\tanh z-a)^2}\right]+r(z) \tag{4.13c}$$

where $r(z)\to 0$ as $z\to+\infty$. Its analytic form is not essential here. From (4.13a, b, c), using (2.3), (2.4) and (4.9) we obtain

$$w^{(1)}(z)=-\mathrm{i}(m-s-p)z+\mathrm{i}\ln G^{(1)},\quad z\to+\infty \tag{4.14a}$$

$$w^{(3)}(z)=\mathrm{i}\ln G^{(3)},\quad z\to+\infty \tag{4.14b}$$

$$w^{(5)}(z)=\mathrm{i}\ln G^{(5)},\quad z\to+\infty \tag{4.14c}$$

where

$$G^{(1)}=\frac{\left(2m-s+\frac{1}{2}\right)^{(1/2)(2m-s+1/2)}}{(m-s-p)^{(m-s-p)}\left(s+\frac{1}{2}\right)^{(1/2)(s+1/2)}}\left(\frac{m+\frac{1}{2}-p}{m+\frac{1}{2}+p}\right)^{(1/2)(m+1/2)}$$

$$\cdot\left[\left(m+\frac{1}{2}\right)^2-p^2\right]^{-p/2} \tag{4.15a}$$

$$G^{(3)}=\exp\left[\frac{1}{48}\left(\frac{1}{m+\frac{1}{2}+p}-\frac{1}{m+\frac{1}{2}-p}+\frac{1}{s+\frac{1}{2}}-\frac{1}{2m-s+\frac{1}{2}}-\frac{4}{m-s-p}\right)\right] \tag{4.15b}$$

$$G^{(5)}=\exp\left[\frac{1}{360}\left(-\frac{7}{16(m+\frac{1}{2}+p)^3}+\frac{7}{16(m+\frac{1}{2}-p)^3}\right.\right.$$

$$-\frac{7}{16(s+\frac{1}{2})^3}+\frac{7}{16(2m-s+\frac{1}{2})^3}-\frac{1}{(m-s-p)^3}\Bigg)\Bigg]. \tag{4.15c}$$

Using Eqs. (3.5), (3.9), (4.12) and (4.15a, b, c), we obtain the phase-integral asymptotic wave function

$$\Psi_S = G\exp[-(m-s-p)z] \tag{4.16}$$

where

$$G=\frac{1}{\sqrt{2\pi x_0}}\sqrt{1+\frac{p}{m-s}}\prod_{n=0}^{N}G^{(2n+1)}. \tag{4.17}$$

Comparing the exact asymptotic formula (2.17) with the phase-integral asymptotic formula (4.17) and (4.15a, b, c) for the normalization factors of the bound states, we see that they are identical. Thus the accuracy of the phase-integral asymptotic expansion is the same as the accuracy of the asymptotic expansion (2.17) in any order of approximation.

In order to show how the accuracy of the phase-integral normalization factors depends on parameters A, B and C and on the order of the phase-integral approximation, we compare numerically the phase-integral result (4.17) with the exact result (2.17). As a measure of the accuracy of the phase-integral normalization factor G we introduce the quantity

$$D=-\log_{10}\frac{|G_e-G|}{G_e} \tag{4.18}$$

equal to a number of significant digits in G. It is valid even when D is not an integer. The number of significant digits D in the phase-integral normalization factor (4.17) in the first-, third- and fifth-order approximation is plotted in Fig. 3a for $B=-144$ and $C=930$ and in Fig. 3b for $B=0$ and $C=930$.

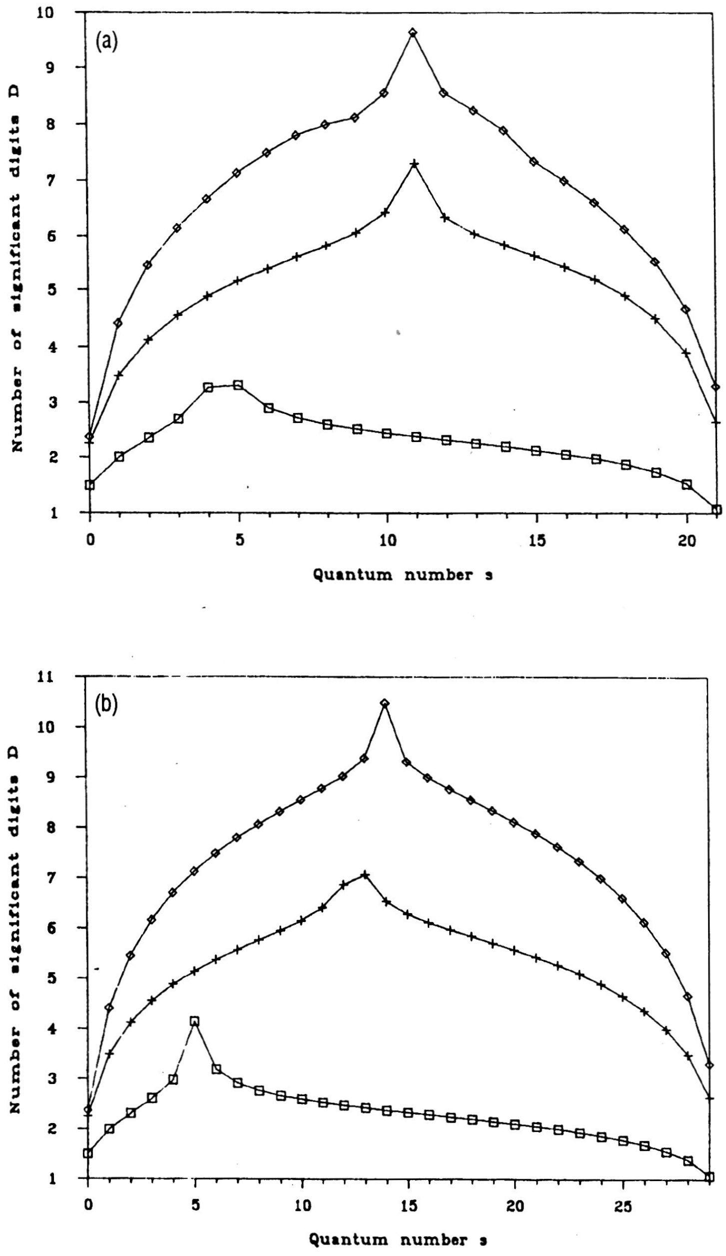

Fig. 3. The number of significant digits D in the phase-integral normalization factor in the first-, third- and fifth-order approximation for $B = -144$ and $C = 930$ as well as for $B = 0$ and $C = 930$. $\square$ First order, $+$ third order, $\diamond$ fifth order.

4.2. The reflexion coefficient

When the square of the base function $Q^2(z)$ is chosen according to (4.1), the similar procedure as in Section 4.1.1. gives the following results for integrals (3.14)

$$K^{(1)} = \pi \left(\sqrt{-c} - \frac{1}{2}\sqrt{a+b-c} - \frac{1}{2}\sqrt{a-b-c} \right), \tag{4.19a}$$

$$K^{(3)} = -\pi \frac{C + \frac{1}{4} - c}{2\sqrt{-c}} + \frac{\pi}{4} \left(\frac{D_+}{\sqrt{a-b-c}} + \frac{D_-}{\sqrt{a+b-c}} \right), \tag{4.19b}$$

$$K^{(5)} = -\pi \frac{(C + \frac{1}{4} - c)^2}{8(-c)^{3/2}} + \frac{\pi}{16} \left(\frac{D_+^2}{\sqrt{(a-b-c)^3}} + \frac{D_-^2}{\sqrt{(a+b-c)^3}} \right). \tag{4.19c}$$

The calculation of the reflexion coefficient for the potential (1.1) has been performed in Ref. 12 when the square of the base function $Q^2(z)$ is chosen equal to the function $R(z)$ appearing in the Schrödinger equation (1.2), i. e., when $a = A$, $b = B$, $c = C$. With such a choice of the base function our results (4.19a, b, c) agree with Eqs. (8) and (9) in Ref. 12.

On the other hand, when a, b and c are chosen according to (4.11), all higher-order contributions ($n = 1,\ 2$) vanish and we obtain from (3.13) and (4.19a, b, c)

$$K = \pi \left(\sqrt{-C - \frac{1}{4}} - \frac{1}{2}\sqrt{A+B-C} - \frac{1}{2}\sqrt{A-B-C} \right), \tag{4.20}$$

in any order of approximation.

In order to compare the numerical results obtained in Ref. 12 with those obtained in the present paper, we write the relations between our parameters A, B, C and parameters W, V_0, V_1 used in Ref. 12 as follows

$$A = 8W - 4V_0 - 2V_1, \quad B = 4V_0, \quad C = -2V_1. \tag{4.21}$$

The numerical example in Table 1 of Ref. 12, where $2 < W < 6$, $V_0 = 1.922$ and $V_1 = 11.2$, corresponds to the case where $-14.088 < A < 17.912$, $B = 7.688$ and $C = -22.4$. The results for the numbers of significant figures in the reflexion coefficient, in the case when $Q^2(z) = R(z)$, for the above values of the parameters W, V_0 and V_1 have been calculated in Ref. 12 up to the eleventh order of approximation. These results are shown in Fig. 1 of Ref. 12.

As a measure of the accuracy of the phase-integral reflexion coefficient, given by (3.12) with (4.20), we introduce the quantity

$$D = -\log_{10} \frac{|R_e - R|}{R_e} \tag{4.22}$$

where R_e is the exact reflexion coefficient given by (2.18). D is a number of significant digits in the phase-integral reflexion coefficient (3.12) with (4.20), valid even when D is not an integer.

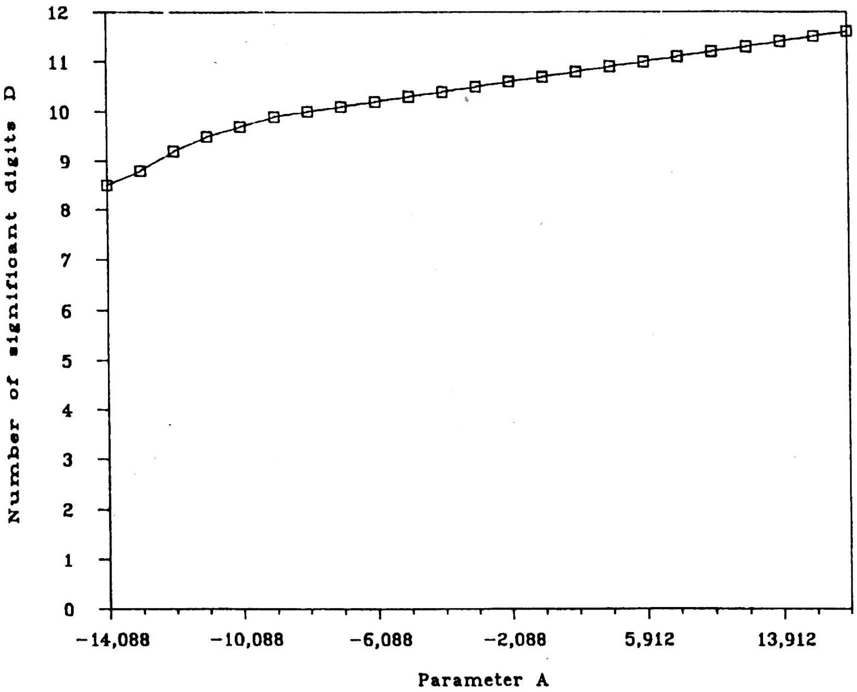

Fig. 4. The number of significant digits D in the phase-integral reflexion coefficient for the transmission of a quantal particle through the potential barrier (1.1) with $-14.088 < A < 17.912$, $B = 7.688$ and $C = -22.4$.

In our Fig. 4 the number of significant digits D of the phase-integral reflexion coefficient R is ploted for the same numerical example as in Fig. 1 of Ref. 12. From Fig. 1 of Ref. 12 and the numerical result presented in our Fig. 4, obtained using our choice of the base function (4.1) with (4.9), we see that the relative error of our phase-integral reflexion coefficient is already in the first-order approximation (in fact in any order of approximation) of the same order of magnitude as the relative error of the eleventh-order phase-integral reflexion coefficient in Ref. 12. The choice of the base function (4.1) with (4.9) corresponds in fact to the case of the infinite-order phase-integral approximation in Ref. 12, as argued in the discussion of the phase-integral quantization condition.

5. *Conclusions*

In conclusion, we note that it was established in Ref. 13 that the first-order phase-integral quantization condition with $Q^2(z)$ chosen according to (4.11) gives the exact bound-state energy in the special case of the symmetric potential (i.e. when $B_0 = 0$). Furthermore it has been shown that the choice of $Q^2(z)$ according to (4.11) is not relevant for the Rosen-Morse potentials only. Choice (4.11) gives the exact, or significantly improved, phase-integral results for all potentials with exponential, hyperbolic and circular functions (e.g. exponential potentials in nuclear models, Morse potential in molecular physics, Pöschl-Teller potentials of first and second type etc.). In the case of circular functions the $\cosh^{-2}(z)$ is of course substituted by $\cos^{-2}(z)$. The unpublished numerical studies indicate that the choice (4.11) gives improved phase-integral results for the three-dimensional case of the centrifugal potential $l(l+1)r^{-2}$ added to any of the above exactly solvable potentials.

It should also be noted that we limit our explicit calculations to the terms with $n = 1,\ 2$ only, due to the increasing complexity. However, by performing the very tedious higher-order calculations, it can be shown that all higher-order ($n = 3,\ 4,\ldots$) contribution to the phase-integral quantization condition consist of one term proportional to $(C+1/4-c)^n$, and a number of terms proportional to $D_\pm^n$, where $D_\pm$ was introduced in (4.8b, c). Thus the choice (4.11) eliminates all higher order contributions to phase integral quantization conditions, and is equivalent to the infinite-order JWKB-approximation for this particular class of potentials. Thus it is expected that the choice (4.11) gives the exact quantization condition for these potentials.

It can also be observed that, using the same choice of the base function $Q^2(z)$, we obtain the exact quantization condition (4.10) with (4.9), while we obtain a very accurate but *NOT* an exact result for the reflexion coefficient (3.12) with (4.25). It is however, a logical and expected result since the phase-integral quantization condition is "asymptotically exact" while the expression for the phase-integral reflexion coefficient is "asymptotically approximate". In other words, even the infinite-order expression for the phase-integral reflexion coefficient is an approximate expression.

Finally, as in the case of the quantization condition, it is possible, although very difficult, to continue the phase-integral calculations of the asymptotic normalization factors (4.17) for $n = 3,\ 4\ldots$ and show that the phase-integral expansion for the normalization factors is also "asymptotically exact".

References

1) N. Rosen and P. M. Morse, Phys. Rev. **42** (1932) 210;

2) M. M. Nieto, Phys. Rev. **A17** (1978) 1273;

3) C. Eckart, Phys. Rev. **35** (1932) 1303;

4) Y. L. Luke, *The Special Functions and their Approximations*, Academic Press Inc., New York, 1969;

5) N. Fröman and P. O. Fröman, *JWKB Approximation*, North-Holland Amsterdam, 1965;

6) N. Fröman and P. O. Fröman, Ann. Phys. (N.Y.) **83** (1974) 103;

7) N. Fröman, Ark. Fys. **32** (1966) 541;

8) N. Fröman, *Semiclassical and Higher-Order Approximations: Properties. Solutions of the Connection Problems.* [In M.S. Child (Ed.), *Semiclassical Methods in Molecular Scattering and Spectroscopy*, 1-44, Redeil publishing Co., (1980)];

9) N. Fröman, Phys. Rev. **A17** (1977) 493;

10) P. O. Fröman, Ann. Phys. (N.Y.) **88** (1974) 621;

11) N. Fröman and P. O. Fröman, Nucl. Phys. **A147** (1970) 606;

12) F. Karlsson, Phys. Rev. **D11** (1975) 2120;

13) C. Rosenzweig and J. B. Krieger, J. Math. Phys. **9** (1968) 849.

RJEŠENJA ZA ROSEN-MORSEOV POTENCIJAL POMOĆU FAZNIH INTEGRALA

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Fazno-integralni uvjet primijenjen je na gibanje kvantne čestice u Rosen–Morseovom potencijalu $V(x) = B_0 \tanh(x/x_0) - U_0 \cosh^{-2}(x/x_0)$. Pokazano je da se uz izbor prikladne valne funkcije dobiva egzaktna vrijednost energije u svim redovima aproksimacije, te da se izraz za normalizacijski faktor zadovoljavajuće podudara s rezultatom egzaktnog računa. Također je pokazano da fazno–integralna formula za koeficijent refleksije daje vrlo točne rezultate.