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Some properties of WKB series

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Abstract. We investigate some properties of the WKB series for arbitrary analytic potentials and then specifically for potentials x^N (N even), where more explicit formulae for the WKB terms are derived. Our main new results are: (i) we find the explicit functional form for the general WKB terms σ_k', where one has only to solve a general recursion relation for the rational coefficients; (ii) we give a systematic algorithm for an essential simplification of the integrated WKB terms $\oint \sigma_k' \, \mathrm{d}x$ that enter the energy eigenvalue equation; and (iii) we derive almost explicit formulae for the WKB terms for the energy eigenvalues of the homogeneous power law potentials $V(x) = x^N$, where N is even.

1. Introduction

Although at present the WKB theory for one-dimensional systems is very thoroughly developed (see, e.g., Delabaere *et al* (1997), Balian *et al* (1979) and Voros (1983)) and its methods are very important for many applications, there are only a few works where the problem of effective calculation of the terms of WKB expansions is discussed. In this direction a pioneering paper is by Bender *et al* (1977), where the authors investigated the structure of the terms of WKB expansions and also applied the methods to compute the eigenvalues of the potential $V(x) = x^N$ (N even positive integer). In our present paper we perform a further study of the problem of the effective computation of WKB series begun in Bender *et al* (1977). We obtain new recurrence formulae for WKB terms for arbitrary analytic potentials, and in particular for the polynomial potential $V(x) = x^N$. The known algorithms are very laborious, because they involve operations of differentiation and collection of similar terms in polynomials, which are extremely time consuming as the order increases, even when modern computer algebra systems are used. In contrast, in computing them by means of our recurrence formulae one performs only arithmetic operations with rational numbers, as we have explicit formulae for the WKB terms, except for the numerical coefficients (exact rational numbers). We also derive almost explicit formulae for the WKB terms for the energy eigenvalues of the homogeneous power law potentials $V(x) = x^N$, where N is even.

These results go substantially beyond the results of Bender *et al* (1977) and indeed it should be emphasized that the main algebraic ideas behind our present work are due to certain remarkable similarities between our present problems and those involved in calculating the normal forms and Lyapunov focus quantities in the power law differential equations (of one degree of freedom) and maps (see Romanovski (1993) and Romanovski and Rauh (1998)). There are also some common features between the problem of reduction of the coefficients σ_k'

of the WKB series and the problem of finding a basis of the ideal of Lyapunov focus quantities (the so-called local 16th Hilbert problem, see Romanovski (1996)). Some introduction to the WKB method can be found in Bender and Orszag (1978).

We consider the two-turning-point eigenvalue problem for the one-dimensional Schrödinger equation

$$\left[-\hbar^2 \frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x). \tag{1}$$

We can always write the wavefunction as

$$\psi(x) = \exp\left\{\frac{1}{\hbar}\sigma(x)\right\} \tag{2}$$

where the phase $\sigma(x)$ is a complex function that satisfies the differential equation

$$\sigma'^2(x) + \hbar\sigma''(x) = (V(x) - E) \stackrel{\text{def}}{=} Q(x). \tag{3}$$

The WKB expansion for the phase is

$$\sigma(x) = \sum_{k=0}^{\infty} \hbar^k \sigma_k(x). \tag{4}$$

Substituting (4) into (3) and comparing like powers of $\hbar$ gives the recursion relation

$$\sigma_0'^2 = Q(x) \qquad \sigma_n' = -\frac{1}{2\sigma_0'}\left(\sum_{k=1}^{n-1} \sigma_k'\sigma_{n-k}' + \sigma_{n-1}''\right). \tag{5}$$

Computing the first few functions σ_k' by means of the recurrent formula we get

$$\sigma_0' = -\sqrt{Q(x)} \qquad \sigma_1' = \frac{-Q'(x)}{4Q(x)} \qquad \sigma_2' = \frac{5Q'(x)^2 - 4Q(x)Q''(x)}{32Q(x)^{\frac{5}{2}}} \tag{6}$$

$$\sigma_3' = \frac{-15Q'(x)^3 + 18Q(x)Q'(x)Q''(x) - 4Q(x)^2 Q^{(3)}(x)}{64Q(x)^4} \tag{7}$$

and

$$\sigma_4' = (1105Q'(x)^4 - 1768Q(x)Q'(x)^2 Q''(x) + 448Q(x)^2 Q'(x)Q^{(3)}(x) \\ +304Q(x)^2 Q''(x)^2 - 64Q(x)^3 Q^{(4)}(x))/2048Q(x)^{\frac{11}{2}}. \tag{8}$$

For the analytical potential $V(x)$ the following quantization condition is known (see Dunham (1932), Fröman and Fröman (1977) and Fedoryuk (1983)):

$$\frac{1}{2i}\oint_\gamma \sum_{k=0}^{\infty} \hbar^k \sigma_k'(x)\, dx = \pi n_q \hbar \tag{9}$$

where $n_q \geqslant 0$ is an integer number and γ is a complex contour enclosing the two turning points on the real axis. This relation is an equation with respect to E and using it one can find the asymptotics of the eigenvalues $E_n(\hbar)$ (see, e.g., Balian *et al* (1979), Fedoryuk (1983) and references therein). In some cases the series (9) can be summed exactly (see Bender *et al* (1977), Robnik and Salasnich (1997a, b), Romanovski and Robnik (1999a, b), Salasnich and Sattin (1997)).

The zero-order term of the WKB expansion is given by

$$\frac{1}{2i}\oint_\gamma d\sigma_0 = \int dx\sqrt{E - V(x)} \tag{10}$$

where the first odd term is

$$\frac{\hbar}{2\mathrm{i}}\oint_{\gamma}\mathrm{d}\sigma_1 = -\frac{\pi\hbar}{2} \tag{11}$$

and to find the higher-order terms we need to compute the functions σ_k' using the recursion relation (5). We note that the odd-order terms (except the first order for σ_1') yield integrals that vanish exactly, because, as follows from the results of Fröman (1966), the functions σ_{2k+1}' are total derivatives.

2. An algorithm for computing σ_k'

We will look for a general formula for the functions σ_k'. As is known, one of the most powerful tools for the investigation of recurrence relations is the method of generating functions (see, e.g., Graham *et al* (1994)). The most widely used in combinatorics generating functions are the ones with a single variable, for example, a generating function for the sequence $\{g_0, g_1, g_2, \ldots\}$ is the formal series

$$G(z) = \sum_{n\geqslant 0} g_n z^n. \tag{12}$$

However, we can also consider a sequence, where every term has only a finite number of indices, but the total number of indices is unbounded (e.g., $g_{(\gamma_1)}, g_{(\gamma_1,\gamma_2)}, g_{(\gamma_1,\gamma_3,\ldots,\gamma_n)}, \ldots$) with the generating function

$$G(z_1, z_2, \ldots) = \sum_{\gamma\in M} g_\gamma \bar{z}^\gamma \tag{13}$$

where $M = \cup_{k=1}^{\infty}\boldsymbol{N}^k$, $\boldsymbol{N}$ is the set of non-negative integers, $\bar{z} = (z_1, \ldots, z_s)$ and $\bar{z}^\gamma = z_1^{\gamma_1}, \ldots, z_s^{\gamma_s}$. Thus in this case $G(z_1, z_2, \ldots)$ is an element of the ring of formal power series in the infinite number of variables, $z_1, z_2, \ldots$. We can consider M as an infinitely dimensional vector space consisting of vectors with only a finite number of coordinates different from zero. If the last non-zero coordinate of $\nu \in M$ is ν_l then we write $\nu = (\nu_1, \ldots, \nu_l)$ instead of $\nu = (\nu_1, \ldots, \nu_l, 0, 0, \ldots)$.

We now apply the method of generating functions to computing the WKB expansion for the phase. Define the map $L : M \to \boldsymbol{N}$ by

$$L(\nu) = 1\cdot\nu_1 + 2\cdot\nu_2 + \cdots + l\cdot\nu_l \tag{14}$$

and denote by $L(\nu) = m$ the equation

$$L(\nu) = 1\cdot\nu_1 + 2\cdot\nu_2 + \cdots + m\cdot\nu_m = m \tag{15}$$

with $m \in \boldsymbol{N}$, $\nu \in M$. For a vector $\nu = (\nu_1, \ldots, \nu_l) \in M$ we denote $Q^{(\nu)} = (Q')^{\nu_1}(Q'')^{\nu_2}\cdots(Q^{(l)})^{\nu_l}$, $|\nu| = \nu_1 + \cdots + \nu_l$ and let $\nu(i)$ $(i = 1, \ldots, l-1)$ be the vector $(\nu_1, \ldots, \nu_i + 1, \nu_{i+1} - 1, \ldots, \nu_l)$. We will show that the functions σ_m' are of the form

$$\sigma_m' = \sum_{\nu:L(\nu)=m} \frac{U_\nu Q^{m-|\nu|}Q^{(\nu)}}{Q^{\frac{3m-1}{2}}} \tag{16}$$

where the coefficients U_ν satisfy the recurrence relation

$$U_\nu = \frac{1}{2}\sum_{\mu,\theta\neq 0,\mu+\theta=\nu} U_\mu U_\theta + \frac{(4 - L(\nu) - 2|\nu|)U_{(\nu_1-1,\nu_2,\ldots,\nu_l)}}{4} + \sum_{i=1}^{l-1}\frac{(\nu_i+1)U_{\nu(i)}}{2} \tag{17}$$

with $U_0 = -1$ and we put $U_\alpha = 0$ if, among the coordinates of the vector α, there is a negative one.

It should be mentioned that the complexity of functions σ'_n increases rapidly with the order n, and it is remarkable that applying our almost explicit formulae (16) and (17) we can go much further than by using the well known recursion relation (5) (see the appendix).

We remind ourselves that a *partition* of the integer number m is a representation of m as a sum of positive numbers, for example, for $m = 4$:

$$4 = 3 + 1 = 2 + 2 = 2 + 1 + 1 = 1 + 1 + 1 + 1. \tag{18}$$

The number of partitions of m is denoted by $p(m)$, in the example above $p(4) = 5$ (there exists a theory and a formula for $p(m)$; see, e.g., Andrews (1976)). It is obvious that there is a one-to-one correspondence between the set of all partitions of m and the set of all solutions ν of the equation (15), $L(\nu) = m$. Therefore as a corollary of formula (16) we find that the number of terms of the function σ'_k cannot exceed $p(m)$. This fact was observed for the first time by Bender *et al* (1977).

We prove the formulae (16) and (17) by induction on m. Indeed, for $m = 1, 2$ the statement holds. Let us suppose that it is true for all $m < k$. Then for $m = k$ we get

$$\frac{\sigma'_i\sigma'_{k-i}}{2\sigma'_0} = \sum_{\theta,\mu:L(\theta)=i,L(\mu)=k-i} -\frac{U_\theta U_\mu Q^{k-|\mu|-|\theta|}Q^{(\mu+\theta)}}{2Q^{\frac{3k-1}{2}}}. \tag{19}$$

Obviously,

$$L(\theta) = i \qquad L(\mu) = k - i \Rightarrow L(\theta + \mu) = k \tag{20}$$

and here we assume that the dimensions of vectors θ and μ are the same. If not, we simply extend the dimension of the smaller one by putting zeros for the excess coordinates. On the other hand, taking into account that all coefficients of the map (14) are positive, it is easy to verify that

$$L(\theta + \mu) = k \Rightarrow L(\theta) = j \qquad L(\mu) = k - j \qquad 0 \leqslant j \leqslant k \tag{21}$$

(this property is the crucial one for the method presented). Thus (19)–(21) yield

$$\sum_{i=1}^{k-1}\frac{\sigma'_i\sigma'_{k-i}}{2\sigma'_0} = \sum_{\theta,\mu:L(\theta+\mu)=k} -\frac{U_\theta U_\mu Q^{k-|\mu|-|\theta|}Q^{(\mu+\theta)}}{2Q^{\frac{3k-1}{2}}} \tag{22}$$

i.e., we get an expression of the form (16).

For the last term of the recurrence formula (5) we get

$$\frac{\sigma''_{k-1}}{2\sigma'_0} = \sum_{\mu:L(\mu)=k-1} -U_\mu\left[\frac{(2-k-2|\mu|)Q^{k-|\mu|-1}Q^{(\mu_1+1,\mu_2,\ldots,\mu_{k-1})}}{4Q^{\frac{3k-1}{2}}} + \frac{Q^{k-|\mu|-1}(Q^{(\mu)})'}{2Q^{\frac{3k-3}{2}}}\right]. \tag{23}$$

Note that for the vector $\mu = (\mu_1, \ldots, \mu_{k-1}, 0)$

$$[Q^{(\mu)}]' = \sum_{i=1}^{k-1}\mu_i Q^{(\hat{\mu}(i))} \tag{24}$$

where we denote by $\hat{\mu}(i)$ $(i = 1, \ldots, k-1)$ the vector $(\mu_1, \ldots, \mu_i - 1, \mu_{i+1} + 1, \ldots, \mu_k)$ $(i = 1, \ldots, k-1)$. It is readily seen that $L(\hat{\mu}(i)) = L(\mu) + 1 = k$; therefore, formulae (5) and (22)–(24) show that (16) and (17) hold.

Using the recurrence relation (17) we can obtain the differential equation for the generating function of the sequence U_ν:

$$U(\bar{z}) = U(z_1, \ldots) = \sum_{\nu\in M} U_\nu \bar{z}^\nu. \tag{25}$$

Let us rewrite (17) in the form

$$U_{(\nu_1,\dots,\nu_l)} = \tfrac{1}{2}\sum_{\mu,\theta\neq 0,\mu+\theta=\nu} U_\mu U_\theta + U_{(\nu_1-1,\nu_2,\dots,\nu_l)} - \tfrac{3}{4}\nu_1 U_{(\nu_1-1,\nu_2,\dots,\nu_l)}$$
$$-\frac{1}{4}\sum_{i=2}^{l}(i+2)\nu_i U_{(\nu_1-1,\nu_2,\dots,\nu_l)} + \sum_{i=1}^{l-1}\frac{(\nu_i+1)U_{\nu(i)}}{2} - [\nu = 0] \tag{26}$$

where $[\alpha = \beta]$ denotes the function, which equals 1 if $\alpha = \beta$ and 0 otherwise.

Using the obvious properties of generating functions (see, e.g., Graham *et al* (1994)) we get from (26)

$$U = \frac{1}{2}(U+1)^2 + z_1 U - \frac{3}{4}z_1(z_1 U)'_{z_1} - \sum_{i=2}^{l}\frac{i+2}{4}z_1 z_i U'_{z_i} + \frac{1}{2}\sum_{i=1}^{l-1} z_{i+1}U'_{z_i} - 1. \tag{27}$$

It means if we fix any integer l and, therefore, the variables $z_1, \dots, z_l$, then the function

$$\hat{U}(z_1, \dots, z_l) = U(z_1, \dots, z_l, 0, 0, \dots) \tag{28}$$

is the solution of equation (27) with the initial conditions

$$\hat{U}(0) = -1 \qquad \hat{U}'_{z_i}(0) = -\frac{1}{2^{i+1}} \tag{29}$$

(we get the initial conditions from (17) taking into account that $U_{(0,\dots,0,1)} = -\frac{1}{2^{i+1}}$ for the vectors with only the ith coordinate different from zero). So, the coefficients U_ν that enter the functions σ'_k (16) are precisely the coefficients of the Taylor expansion of the function $\hat{U}$ defined by the differential equation (27) with the initial conditions (29).

Coefficients of the form $U_{(n,0,\dots,0)} \stackrel{\text{def}}{=} U_n$ depend on the coefficients of the same form. Therefore we get from (27) that the function $U(z) = \sum_{n=0}^{\infty} U_n z^n$ satisfies the differential equation

$$U = \tfrac{1}{2}(U+1)^2 + zU - \tfrac{3}{4}z(zU)'_z - 1 \tag{30}$$

which is the Riccati equation

$$3z^2 U'_z - 2U^2 - zU + 2 = 0. \tag{31}$$

Note that as an immediate corollary of formula (16) we get that for the harmonic oscillator, i.e. when $Q = x^2 - E$, the WKB series (9) terminates after the first two terms, namely

$$\oint_\gamma \mathrm{d}\sigma_k = 0 \tag{32}$$

for all $k \geqslant 2$. Indeed, in this case (16) yields

$$\sigma'_m = \sum_{i=0}^{[m/2]} \frac{U_{(m-2i,i)}2^{m-i}x^{m-2i}}{\sqrt{x^2-E}^{3m-1-2i}} \tag{33}$$

where $[m/2]$ stands for the integer part of $m/2$.

It is obvious

$$\mathrm{Res}_\infty \frac{x^{m-2i}}{\sqrt{x^2-E}^{3m-1-2i}} = 0 \tag{34}$$

for all $m > 1$. Therefore (32) takes place.

3. An algorithm for the simplification of the functions $\mathrm{d}\sigma_k$

It was pointed out by Bender *et al* (1977) that the functions $\mathrm{d}\sigma_k$ can be dramatically simplified by adding and subtracting total derivatives (obviously, such an operation does not change the integrals (9)). They also carried out numerical experiments to obtain different simplifications of these functions. It is easily seen that formula (16) provides an effective way to reduce the number of terms in the expressions for the functions $\mathrm{d}\sigma_k$.

We will look for a function of the form

$$P_{k-1} = \sum_{\mu:L(\mu)=k-1} \frac{W_\mu Q^{k-1-|\mu|} Q^{(\mu)}}{Q^{\frac{3k-3}{2}}} \tag{35}$$

where W_μ are to be determined, such that

$$\frac{\mathrm{d}}{\mathrm{d}x} P_{k-1} = \sigma_k'. \tag{36}$$

If equation (35) has a solution, then σ_k' is a total derivative of the function P_{k-1} and then the contour integral $\oint \mathrm{d}\sigma_k$ vanishes. However, if (35) has no solution, we can still use it in order to eliminate (subtract) as many terms as possible in the expression $\mathrm{d}\sigma_k$, which is then replaced by $\mathrm{d}\hat{\sigma}_k$ (see equation (38)).

By comparing coefficients of $\frac{Q^{k-|\nu|} Q^{(\nu)}}{Q^{\frac{3k-1}{2}}}$, in both parts of (36) we get the system of linear equations of unknown variables W_μ:

$$\frac{3 - L(\nu) - 2|\nu|}{2} W_{(\nu_1-1,\nu_2,\ldots,\nu_l)} + \sum_{i=1}^{l-1} (\nu_i + 1) W_{\nu(i)} = U_\nu \tag{37}$$

where $\nu = (\nu_1, \ldots, \nu_l)$ runs through the whole set of solutions of equation $L(\nu) = k$ and U_ν are defined by the recurrence relations (16) and (17). Thus to simplify the function $\mathrm{d}\sigma_k$ one can use the system (37) of $p(k)$ equations in $p(k-1)$ variables W_μ.

Let us denote by $\tilde{p}(k)$ the number of partitions of k which contain at least one 1. Obviously, $p(k) = \tilde{p}(k+1)$. It appears that the optimal strategy to simplify σ_k' is as follows. In system (37), where $L(\nu) = k$ for U_ν on the right-hand side, we consider the equations with ν such that $\nu_1 \neq 0$. There are $\tilde{p}(k) = p(k-1)$ such equations and, according to (35), we have exactly $p(k-1)$ variables W_μ. It turns out that we can always write the systems with U_ν such that $\nu_1 \neq 0$ in the triangular form (like system (39) below). To see this we set the following order on vectors of M: we say that $\nu < \mu$ if the first nonzero entry from the left in $\mu - \nu$ is positive (this order is known in computational algebra as the lexicographic one). Then if we write down the equations of system (37), corresponding to $U_{\nu^{(1)}}, U_{\nu^{(2)}}, \ldots$ in decreasing order $\nu^{(1)} > \nu^{(2)}, \ldots$ and the variables W_μ in these equations also in decreasing order then we find that the matrix corresponding to the first $p(k-1)$ equations is the triangular $p(k-1) \times p(k-1)$ matrix (because $\nu(i) > (\nu_1 - 1, \nu_2, \ldots, \nu_l)$ for $1 \leqslant i \leqslant l-1$). We denote this triangular $p(k-1) \times p(k-1)$ matrix by B and the whole system (37) by $A \cdot w = u$, where w is the ordered vector of variables W_μ, u is the ordered vector of U_ν and A is the matrix of the linear system (37). Let u_1 be the $p(k-1)$ vector such that its coordinates coincide with the first $p(k-1)$ coordinates of the vector u. The diagonal elements of the matrix B are equal to $(3 - L(\nu) - 2|\nu|)/2$ and, hence, are different from zero. Therefore the system $B \cdot w = u_1$ has the solution w^* and using the vector $u - A \cdot w^*$ we obtain the simplified function

$$\hat{\sigma}_k'(x) = \sigma_k'(x) - \frac{\mathrm{d}}{\mathrm{d}x} P_{k-1} \tag{38}$$

such that $\oint_\gamma \mathrm{d}\sigma_k = \oint_\gamma \mathrm{d}\hat{\sigma}_k$. Hence, we see that after the simplification $\mathrm{d}\sigma_{2n}$ contains at most $p(2n) - p(2n-1)$ terms.

For example, to simplify $d\sigma_4$ we write down the corresponding system (37) and get

$$\begin{array}{lcl} U_4 & = & -\frac{9}{2}\, W_3 \\ U_{(2,1)} & = & 3\, W_3 - \frac{7}{2}\, W_{(1,1)} \\ U_{(1,0,1)} & = & W_{(1,1)} - \frac{5}{2}\, W_{(0,0,1)} \\ U_{(0,2)} & = & W_{(1,1)} \\ U_{(0,0,0,1)} & = & W_{(0,0,1)} \end{array} \tag{39}$$

where $U_4 = 1105/2048$, $U_{(2,1)} = -1768/2048$, $U_{(0,2)} = 304/2048$, $U_{(1,0,1)} = 448/2048$, $U_{(0,0,0,1)} = -64/2048$. For this case $w = (W_3, W_{(1,1)}, W_{(0,0,1)})^\top$, $u = (U_4, U_{(2,1)}, U_{(1,0,1)}, U_{(0,2)}, U_{(0,0,0,1)})^\top$, $u_1 = (U_4, U_{(2,1)}, U_{(1,0,1)})^\top$. Solving the system $B \cdot w = u_1$, which in this case is the system of the first three equations of (37) (note that the matrix, corresponding to these equations, is the triangular one), we find

$$W_3 = -\tfrac{1105}{9216} \qquad W_{(1,1)} = \tfrac{221}{1536} \qquad W_{(0,0,1)} = -\tfrac{23}{768}. \tag{40}$$

Hence

$$u - A \cdot w^* = (0, 0, 0, \tfrac{7}{1536}, -\tfrac{2}{1536}) \tag{41}$$

where A is the matrix of system (39). It means that

$$\hat{\sigma}_4' = \sigma_4' - \frac{d}{dx} P_3 = \frac{7Q''(x)^2 - 2Q(x)Q^{(4)}(x)}{1536 Q(x)^{7/2}} \tag{42}$$

in accordance with Bender *et al* (1977).

To end this section we show that in some cases we can replace calculation of the contour integral by computing a Riemann integral, namely we shall show that formula (44) below applies.

First we note that taking into account that $Q = V(x) - E$ we can write formula (16), for even m, in the form

$$\sigma_m' = \sum_{\nu:L(\nu)=m} \frac{2^{\frac{m}{2}-1+|\nu|}\, \mathrm{i}}{(m-3+2|\nu|)!!} \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \frac{U_\nu V^{(\nu)}}{\sqrt{E-V}}. \tag{43}$$

Let us now suppose that $Q = V(x) - E$, where $V(x)$ is an analytic function with one minimum and $V'(x) \neq 0$, if $x \neq 0$. We will show that

$$\oint d\sigma_m = 2 \sum_{\nu:L(\nu)=m} \frac{2^{\frac{m}{2}-1+|\nu|}\, \mathrm{i}}{(m-3+2|\nu|)!!} \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \int_{x_1}^{x_2} \frac{U_\nu V^{(\nu)}}{\sqrt{E-V}}\, dx \tag{44}$$

where $V(x_1) = V(x_2) = E_0$, $x_1 < x_2$. Taking into account (43) it is easy to see that to prove (44) it is sufficient to show that

$$\oint_\gamma \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \frac{V^{(\nu)}}{\sqrt{E-V}}\, dx = 2 \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \int_{x_1}^{x_2} \frac{V^{(\nu)}}{\sqrt{E-V}}\, dx. \tag{45}$$

Note that, due to the theorem on differentiation upon a parameter (see, e.g., Sidorov *et al* (1976)), if

$$F(E) = \oint_\gamma f(x, E)\, dx \tag{46}$$

and

(1) γ is a finite piecewise-smooth curve;
(2) the function $f(x, E)$ is continuous with respect to (x, E) for $x \in \gamma$, $E \in D$, where D is a domain of the complex plane;

(3) for every fixed $x \in \gamma$ the function $f(x, E)$ is analytic upon E in D, then $F(E)$ is analytic in D and

$$F'(E) = \oint_\gamma \frac{\partial f(x, E)}{\partial E}\, \mathrm{d}x \tag{47}$$

for $E \in D$.

Let us cut the complex plane between the turning points x_1 and x_2 to get a single-valued function and fix the contour $(x_1 + \rho, x_2 - \rho) \cup c_1 \cup (x_2 - \rho, x_1 + \rho) \cup c_2$, where ρ is small, c_1, c_2 are circles: $c_1 = x_2 + \rho \mathrm{e}^{\mathrm{i}t}$, $c_2 = x_1 + \rho \mathrm{e}^{\mathrm{i}t}$ and $t \in [0, 2\pi]$. Then the conditions (1)–(3) are satisfied (with D being a small neighbourhood of E_0). Therefore

$$\oint_\gamma \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \frac{V^{(\nu)}}{\sqrt{E-V}}\, \mathrm{d}x = \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \oint_\gamma \frac{V^{(\nu)}}{\sqrt{E-V}}\, \mathrm{d}x$$
$$= \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \left(2\int_{-x_0+\rho}^{x_0-\rho} \frac{V^{(\nu)}}{\sqrt{E-V}}\, \mathrm{d}x + \oint_{c_1} \frac{V^{(\nu)}}{\sqrt{E-V}}\, \mathrm{d}x + \oint_{c_2} \frac{V^{(\nu)}}{\sqrt{E-V}}\, \mathrm{d}x \right). \tag{48}$$

Let us denote

$$g(E) = \oint_{c_1} \frac{V^{(\nu)}}{\sqrt{E-V}}\, \mathrm{d}x. \tag{49}$$

Due to the theorem mentioned above $g(E)$ is analytic in a neighbourhood of E_0. Therefore

$$g(E) \approx g(E_0) + g'(E_0)(E - E_0). \tag{50}$$

Noting that

$$|g(E_0)| = \left| \oint_{c_1} \frac{V^{(\nu)}}{\sqrt{E_0 - V}}\, \mathrm{d}x \right| = \left| \oint_{c_1} \frac{V^{(\nu)}}{\sqrt{V'(x_1)(x - x_1) + \cdots}}\, \mathrm{d}x \right| < \text{ const } \rho^{1/2} \tag{51}$$

we obtain that $g(E) \to 0$ when $\rho \to 0$, $E \to E_0$. It means that formula (45) indeed holds. This formula has been found useful for computing the WKB series for the Coulomb potential and the potential $V(x) = U_0/\cos^2(\alpha x)$ (Robnik and Salasnich 1997a, b).

4. Potentials of the form $V(x) = x^N$

In recent decades many studies have been devoted to the investigation of the semiclassical expansions for potentials of the form $V(x) = x^N$ and important results have been achieved (see, e.g., Balian *et al* (1979), Voros (1983) and references therein).

One of the basic formulae for these potentials was obtained by Bender *et al* (1977) and is as follows:

$$\pi(n_q + \tfrac{1}{2}) = E^{1/N+1/2} \sum_{n=0}^{\infty} E^{-n(1+2/N)} a_n(N) \tag{52}$$

where N is an even integer number,

$$a_n(N) = \frac{(-1)^n 2^{1-n} \sqrt{\pi}\, \Gamma(1 + \frac{1-2n}{N}) P_n(N)}{(2+2n)!\, \Gamma(\frac{3-2n}{2} + \frac{1-2n}{N})} \tag{53}$$

and $P_n(N)$ are polynomials of the variable N with integer coefficients, in particular $P_0(N) = 1$, and therefore $a_0(N) = \frac{\sqrt{\pi}\Gamma(1+\frac{1}{N})}{\Gamma(\frac{3}{2}+\frac{1}{N})}$. The first eight polynomials $P_n(N)$ were computed using the MACSYMA computer algebra program by Bender *et al* (1977) for the general potential $V(x) = x^N$ and, as was mentioned, the computation of the eighth polynomial has already faced difficulties. When N is a fixed numerical integer number then, instead of the polynomials a_n, we have integers. The special case of the quartic oscillator ($N = 4$) has been investigated by Balian, Parisi, Voros and others. In this case the expression of the type (52) is written (Balian *et al* 1979) in the form

$$2\pi(n_q + \tfrac{1}{2})\hbar = \sum_{n=0}^{\infty} b_n \sigma^{1-2n} \hbar^{2n} \tag{54}$$

where

$$\sigma = E^{3/4} B(\tfrac{3}{2}, \tfrac{1}{4}) \tag{55}$$

is the classical action around the closed orbit of energy E (here $B(x, y)$ is the beta function) and b_n in this case are rational numbers. As is reported by Balian *et al* (1979) using the REDUCE language they were able to compute the first 17 coefficients b_n. Then they had to switch to ordinary numerical computation and computed b_n up to $n = 53$ (in Voros (1983) the results of computation up to $n = 60$ are presented).

It was mentioned in Balian *et al* (1979) and Bender *et al* (1977) that the authors do not know any closed form or simple law for the coefficients $a_n(N)$ and b_n. In this section we partially answer this question. Although we also were not able to find any closed form for the functions a_n (or numbers b_n) we obtain a simple recurrence formula, where only operations of summation and multiplication of rational numbers are involved, whereas using the usual method of the above-mentioned papers one needs first to compute rational functions of the form $f(x, \sqrt{E - x^N})$ and then evaluate contour integrals. We carried out computer experiments and found out that using our algorithm with Mathematica 4.0 on a PC with 128 MB RAM we were able to compute in closed arithmetic form the coefficients b_n at least up to $n = 190$ for the quartic potential (see also the appendix).

It can be proven (Robnik and Romanovski 2000) by induction using the recursion relation (5) that for the potential $V(x) = x^N$ the coefficients σ'_k ($k \geqslant 1$) of the WKB expansion have the form

$$\sigma'_k = -\frac{(-\mathrm{i})^{3k-1} x^{-k+N}}{(E - x^N)^{\frac{3k-1}{2}}} \sum_{j=0}^{k-1} A_{k-j-1,j} E^{k-j-1} x^{jN} \tag{56}$$

where we choose $\sqrt{E - x^n} = \mathrm{i}\sqrt{x^n - E}$, and the coefficients $A_{k-j-1,j}$ of the monomials $E^{k-j-1} x^{jN}$ are computed according to the recurrence formula

$$A_{s,l} = \frac{1}{2} \sum_{i=0}^{s} \sum_{j=0}^{l-1} A_{i,j} A_{s-i,l-1-j} + \frac{l(2+N) + (2+3N)s - N}{4} A_{s,l-1} + \frac{(N-1)l + N - s}{2} A_{s-1,l}. \tag{57}$$

with $A_{0,0} = \frac{N}{4}$ and

$$A_{\alpha,\beta} = 0 \qquad \text{if} \quad \alpha < 0 \qquad \text{or} \qquad \beta < 0. \tag{58}$$

Using equation (57) we can get the differential equation for the generating function of the coefficients $A_{s,l}$, and in the special case $A_{s,0}$ one can find the explicit formula (Robnik and Romanovski 2000)

$$A_{s,0} = \frac{N!}{2^{s+2}(N - s - 1)!}. \tag{59}$$

For even k, ($k \leftrightarrow 2k$) we can write formula (56) in the form

$$\sigma'_{2k} = \sum_{j=0}^{2k-1} \frac{\mathrm{i}2^{3k}}{(6k-3)!!} A_{2k-j-1,j} E^{2k-j-1} x^{-2k+(j+1)N} \frac{\partial^{3k}}{\partial E^{3k}} (E - x^N)^{1/2}. \tag{60}$$

As above we can replace the integration on a contour with the integration between turning points. Then, taking into account that

$$\int_0^a x^{\alpha-1}(a^\theta - x^\theta)^{\beta-1}\,\mathrm{d}x = \frac{a^{\theta(\beta-1)+\alpha}}{\theta} B\left(\frac{\alpha}{\theta}, \beta\right) \tag{61}$$

where $\alpha, \theta, \mathrm{Re}\,\alpha, \mathrm{Re}\,\beta > 0$, and B is the beta function, and noting that

$$\frac{\Gamma(\frac{3}{2} + s + \frac{1-2k}{N} + 1)}{\Gamma(\frac{3}{2} + s + \frac{1-2k}{N} - 3k)} = \left(\frac{3}{2} + s + \frac{1-2k}{N}\right) \times \left(\frac{3}{2} + s + \frac{1-2k}{N} - 1\right)\cdots\left(\frac{3}{2} + s + \frac{1-2k}{N} - 3k\right) \tag{62}$$

we get from (60)

$$\oint_\gamma \mathrm{d}\sigma_{2k} = 2\int_{-E^{1/n}}^{E^{1/n}} \mathrm{d}\sigma_{2k} = \frac{2^{3k+1}\mathrm{i}\sqrt{\pi}}{(6k-3)!!N} E^{\frac{1}{2}+\frac{1}{N}} \sum_{s=0}^{2k-1} A_{2k-s-1,s} E^{-\frac{2k}{N}-k} \frac{\Gamma(\frac{1-2k}{N} + s + 1)}{\Gamma(\frac{3}{2} + s + 1 - 3k + \frac{1-2k}{N})} \tag{63}$$

and using the equality $\Gamma(1 + z) = z\Gamma(z)$ we finally obtain the coefficients of the WKB expansion:

$$\oint_\gamma \sigma'_{2k}\,\mathrm{d}x = \frac{\mathrm{i}2^{3k+1}\sqrt{\pi}}{(6k-3)!!N} E^{\frac{1}{2}+\frac{1}{N}-\frac{2k}{N}-k} \frac{\Gamma(\frac{1-2k}{N}+1)}{\Gamma(\frac{3-2k}{2}+\frac{1-2k}{N})} \times\left(A_{2k-1,0}\prod_{s=1}^{2k-1}\left(\frac{3-2k}{2} + \frac{1-2k}{N} - s\right) + \sum_{i=1}^{2k-1} A_{2k-i-1,i}\prod_{s=1}^{i}\left(s + \frac{1-2k}{N}\right) \times \prod_{s=1}^{2k-i-1}\left(\frac{3-2k}{2} + \frac{1-2k}{N} - s\right)\right) \tag{64}$$

where $k \geqslant 1$ and $A_{2k-i-1,i}$ are computed according to (57) and

$$\oint_\gamma \sigma'_0\,\mathrm{d}x = \frac{2\mathrm{i}E^{\frac{1}{2}+\frac{1}{N}}\sqrt{\pi}\Gamma(1+\frac{1}{N})}{\Gamma(\frac{3}{2}+\frac{1}{N})}. \tag{65}$$

5. Conclusions

To conclude, in this paper we have investigated the WKB approximations as a series for arbitrary analytic potentials. In particular, we obtain effective algorithms to compute and reduce the terms of these series. In computing by means of these formulae we manipulate only with *numbers* and do not need to collect similar terms of a polynomial, which we must do otherwise when we use just the recursion formula (5). Application of the formulae obtained along with the reduction formula (37) considerably simplifies calculations, especially if we need to compute higher-order terms. We also derive simple formulae for the WKB terms for the energy eigenvalues of the polynomial potentials $V(x) = x^N$, where N is even.

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Table A.1. (a) The order n of the coefficient σ_n', (b) the number of terms in the coefficient σ_n' ($= p(n)$), (c) CPU time in seconds for computing σ_n' by means of formula (5), (d) CPU time for computing σ_n' using formulae (16) and (17).

(a)	(b)	(c)	(d)	(a)	(b)	(c)	(d)
10	42	0.47	0.54	30	5 604	18 542	1 402
15	176	5.7	5.2	34	12 310	114 219	4 981
20	627	83	41	35	14 883	—	6 733
25	1958	1509	256	40	37 338	—	29 940

Table A.2. $V(x) = x^4$.

n	A_n
53	$0.994\,978\,900\,682\,695\,793\,998\,335\,252\,220\,4\underline{201}$
54	$-0.995\,073\,373\,044\,872\,143\,603\,833\,247\,793\,08\underline{91}$
55	$0.995\,164\,356\,634\,546\,100\,730\,933\,541\,912\,349\underline{5}$
56	$-0.995\,252\,041\,172\,171\,612\,549\,261\,251\,302\,2\underline{471}$
57	$0.995\,336\,602\,869\,245\,232\,422\,036\,639\,4\underline{79\,6240}$
58	$-0.995\,418\,205\,609\,461\,232\,694\,905\,9\underline{32\,439\,4196}$
59	$0.995\,497\,002\,008\,086\,630\,872\,9\underline{69\,891\,605\,0341}$
60	$-0.995\,573\,134\,363\,955\,136\,819\,952\,539\,7\underline{20\,4894}$

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Appendix

Here we present the results of computer experiments which we carried out with Mathematica 4.0 on our PC with a 450 MHz processor and 128 MB RAM to compare the efficiency of our algorithms based on equations (16), (17), (57) and (64) with traditional ones.

To compute σ_n' by Mathematica using formula (5) one can just use it in the form presented in the text, but for computing by means of formulae (16) and (17) a procedure has to be written.

In the case of the potential $V(x) = x^4$ for computing $\oint \sigma_{2n}' \, \mathrm{d}x$ one can use formulae (57) and (64) precisely in the form presented in this paper, but it is a necessary preliminary to define $A_{-1,i} = A_{i,-1} = 0$.

In Voros (1983) the table of results of numerical calculations of the numbers

$$A_n = \frac{2^{-\frac{3}{2}-n} \pi b_n \csc(\frac{(3-6n)\pi}{4})}{\Gamma(2n-1)}$$

(which should not be confused with our $A_{s,l}$ and where the numbers b_n are defined in equation (54), with an estimated accuracy of 34 digits) are presented and it is mentioned there that the accuracy is not guaranteed for n close to 60. Indeed, we found perfect correspondence with the table of Voros (1983) up to $n = 52$. However, for larger n there is disagreement with our calculations, presented in table 2 (digits which differ from those obtained by Voros (1983) are underlined). It should be emphasized that here we calculate A_n in the exact arithmetic form, which includes rational numbers and the gamma function, but show here the numerical results just for the purpose of comparing them with those of Voros (1983).

We computed the coefficients b_n in exact arithmetic form according to formulae (57) and

(64) up to $n = 190$ and it took 143 555 s CPU time to do so. It was possible to continue computations according to the memory capacity. However, the computations became too time consuming. As is reported by Balian *et al* (1979) using the REDUCE language they were able to go up to $n = 16$.

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