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Numerological analysis of the WKB approximation in large order

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We show how to solve the one-dimensional two-turning-point eigenvalue problem for analytic potentials to *all orders* in the WKB approximation. We use this method to compute the eigenvalues of the x^N (N even) potential to twelfth order. Numerical results for the x^4 potential are accurate to 1 part in 10^{15} for the tenth eigenvalue. For the $\nu_0 \cosh^{-2}x$ potential the WKB series reduces to a geometric series which may be summed to give the exact answer. Finally, we report on the results of numerological experiments on the structure of the WKB series. The simplicity of our results leads us to conjecture (weakly) that it may be possible to find a formula for the terms of the WKB series for arbitrary analytic potentials.

I. EXACT WKB QUANTIZATION CONDITION

In this paper we consider the two-turning-point eigenvalue problem for the one-dimensional Schrödinger equation

$$\left[\frac{-d^2}{dx^2} + V(x) - E\right] y(x) = 0, \quad y(\pm\infty) = 0\,. \tag{1}$$

For simplicity, we assume here that the potential $V(x)$ is a one-valued analytic function which is real on the real axis, that $V(\pm\infty) = \infty$, that $V(x)$ has a unique minimum somewhere along the real axis, and that $V(x)$ rises monotonically on both sides of the minimum so that $V(\pm\infty) = \infty$. Widely studied potentials like $V(x) = x^4$, x^{2N} ($N = 1, 2, \ldots$), $\cosh x$ satisfy these criteria. Potentials of this type give rise to an infinite nondegenerate spectrum of energy eigenvalues $E^{(K)}$, $K = 0, 1, 2, \ldots$.

It is commonly known that the WKB approximation provides a good leading-order approximation to the eigenvalues $E^{(K)}$ when K is large. The standard two-turning-point analysis predicts that the implicit relation

$$\int_{x_1}^{x_2} [E - V(x)]^{1/2}\, dx = (K + \tfrac{1}{2})\pi \quad (K = 0, 1, 2, \ldots) \tag{2}$$

becomes exact as $K \to \infty$. [x_1 and x_2 are called turning points; they are the two places where the potential energy $V(x)$ equals the total energy E.] Equation (2) is a convenient formula for calculating the approximate values of $E^{(K)}$.

It is not generally known, however, that there is a better formula, almost as simple as (2), which can be used to calculate the eigenvalues to *any* order in the WKB approximation. To construct this formula we introduce a small parameter ϵ into (1) and consider the eigenvalue problem

$$\epsilon^2 y''(x) = Q(x) y(x), \quad y(\pm\infty) = 0\,, \tag{3}$$

where

$$Q(x) = V(x) - E\,.$$

The parameter ϵ helps to organize the WKB series; we set $\epsilon = 1$ when the calculation is completed. The WKB approximation for the wave function $y(x)$ is

$$y(x) = \exp\left[\frac{1}{\epsilon} \sum_{n=0}^{\infty} \epsilon^n S_n(x)\right]\,. \tag{4}$$

Substituting (4) into (3) and comparing like powers of ϵ gives expressions for $S_n'(x)$:

$$S_0'(x) = -[Q(x)]^{1/2}\,, \tag{5}$$

$$2S_0' S_n' + \sum_{j=1}^{n-1} S_j' S_{n-j}' + S_{n-1}'' = 0 \quad (n \geq 1)\,. \tag{6}$$

The recursion relation in (6) is a simple algebraic rule for computing $S_n'(x)$ from S_j' for $j < n$. Straight calculation gives

$$S_1'(x) = \frac{-Q'(x)}{4Q(x)}\,, \tag{7}$$

$$S_2'(x) = \frac{5[Q'(x)]^2}{32[Q(x)]^{5/2}} - \frac{Q''(x)}{8[Q(x)]^{3/2}}\,, \tag{8}$$

$$S_3'(x) = \frac{-15[Q'(x)]^3}{64[Q(x)]^4} + \frac{9Q'(x)Q''(x)}{32[Q(x)]^3} - \frac{Q'''(x)}{16[Q(x)]^2}\,, \tag{9}$$

and so on.

Once the S_n' have been found, there is a simple formula, which is a generalization of (2) to all orders in the WKB approximation, which states the *exact* quantization of the eigenvalues:

$$\frac{1}{2i} \oint \sum_{n=0}^{\infty} S_n'(z)\, dz = K\pi \quad (K = 0, 1, 2, \ldots)\,, \tag{10}$$

where we have now set $\epsilon = 1$. The integral in (10) is a complex contour integral which encircles the two turning points on the real axis. This beautiful formula, which was first written in this form by Dunham,[1] is the basis of our paper.

Let us see how formula (10) reduces to the leading-order WKB approximation in (2). The leading-order WKB approximation (physical optics) takes into account both $S_0(x)$ and $S_1(x)$. [Geometrical optics only deals with $S_0(x)$.] Substituting $S_0'(x)$ in (5) into (10) and making $[Q(z)]^{1/2}$ single valued by joining the turning points at x_1 and x_2 by a branch cut gives

$$\frac{1}{2i}\oint -[V(z)-E]^{1/2}dz=\int_{x_1}^{x_2}[E-V(x)]^{1/2}dx\,,$$

and substituting S_1' in (7) into (10) gives

$$\frac{1}{2i}\oint -\frac{Q'(z)}{4Q(z)}dz=-\frac{1}{8i}\ln Q(z)\Big|_{\text{evaluated once around the contour}}$$

$$=-\frac{1}{8i}4\pi i=-\frac{\pi}{2}\,.$$

[Evaluating $\ln Q(z)$ once around the contour gives $4\pi i$ because the contour encircles two simple zeros of $Q(z)$ at x_1 and x_2.] Substituting these results into (10) reproduces the leading-order approximation in (2).

Let us consider the structure of the exact quantization condition in (10). It is remarkable that while (10) may be derived using turning-point analysis and asymptotic matching to all orders, all reference to Airy functions has dropped out. Moreover, there is no reference to the wave function $y(x)$ or to its boundary conditions $y(\pm\infty)=0$. The construction of the integrand in (10) is a purely *algebraic* procedure involving differentiation but not integration. It is necessary to use complex contour integration in place of ordinary intergration along the real axis from x_1 to x_2 because the functions $S_2'(x), S_3'(x), \ldots$ are singular at the turning points x_1 and x_2. All the contour integrals in (10) of the form $\oint S_n'(z)dz$ exist for all n.

Our purpose in writing this paper is twofold. First, we demonstrate how to calculate eigenvalues very accurately with (10). For example, by going to twelfth order in the WKB approximation we can calculate $E^{(10)}$ for $V=x^4$ accurately to better than 2 parts in 10^{15}. Moreover, we can use (10) to calculate the eigenvalues of some potentials exactly: We show why the lowest-order WKB approximation for the harmonic oscillator gives the exact eigenvalues [the series in (10) truncates after the first two terms[2]]. For certain other potentials like $\cosh^{-2}x$ the series in (10) becomes a geometric series which sums to give the exact answer.

Our second objective is to raise an interesting question which we are as yet unable to answer. Because the integrals in (10) all involve closed contours, it is possible to add total derivatives to $S_n'(z)$ under the integral sign without altering the value of the integral. Thus, S_n', as generated by the recursion relation in (6), is but one element of a large equivalence class which we denote by E_n. The elements of E_n are all different but their contour integrals are all identical. Is it possible that for all n there is some element of E_n which is so simple that the indicated sum in (10) may be evaluated in closed form? If so, we will have achieved an exact closed-form implicit condition for the eigenvalues of the Schrödinger operator with any analytic potential.

This possibility is quite remote, but we have carried out some algebraic experiments which continue to buoy our hopes. For example, it is interesting that one element of E_{2n+1}, $n\geq 1$, is always 0 because S_{2n+1}', $n\geq 1$, is itself a total derivative. For example, $S_3'(x)$ in (9) may be rewritten as

$$S_3'(x)=\frac{d}{dx}\left\{\frac{5[Q'(x)]^2}{64[Q(x)]^3}-\frac{Q''(x)}{16[Q(x)]^2}\right\},$$

which vanishes when integrated along the closed contour in (10).[3] Thus, (10) immediately simplifies to a sum over even-numbered terms only[4]:

$$\frac{1}{2i}\oint\sum_{n=0}^{\infty}S_{2n}'(z)dz=(K+\tfrac{1}{2})\pi\quad(K=0,1,2,\ldots)\,. \tag{11}$$

We have also found that S_{2n}' can be dramatically simplified by adding and subtracting total derivatives. For example, $S_2'(x)$ in (8) may be written as *one* term minus a total derivative

$$S_2'(x)=-\frac{Q''(x)}{48[Q(x)]^{3/2}}-\frac{d}{dx}\left\{\frac{5Q'}{48[Q(x)]^{3/2}}\right\};$$

the total derivative integrates to zero because the function in large curly brackets is a single-valued function of z on the contour of integration when the turning points are joined by a branch cut. However, we are not yet able to guess complete closed closed-form expressions for simple elements of E_{2n}.

There is a very close parallel between our search for a simple element of E_{2n} and the construction of the conserved quantities for nonlinear wave equations like the Korteweg-de Vries equation. For this equation the conserved quantities are derived from the Bäcklund transformation

$$u(x)=-v^2(x)-\frac{dv}{dx}$$

and the conserved densities (to which one may add or subtract total derivatives) satisfy a recursion relation like that in (7).[5] In this paper, the recursion relation in (7) for the elements S_n' of the WKB expansion may be derived from the Bäcklund transformation if we take $u=v/\epsilon$ and let $v=\sum_0^\infty \epsilon^n S_n'$.

The Bäcklund transformation is just the Riccati equivalent of the Schrödinger equation.

This paper is organized as follows. In Sec. II we give the results of using (11) to twelfth order in the WKB approximation for potentials of the form $V(x)=x^N$ $(N=2,4,6,\ldots)$, and we discuss special potentials in which the series in (11) may be summed exactly. In Sec. III we discuss (11) on a rather numerological level and suggest various approaches for finding a closed-form expression for elements of E_{2n}.

II. APPLICATION OF THE QUANTIZATION CONDITION IN (11) TO SPECIFIC POTENTIALS

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

We used the MACSYMA computer program at MIT to perform the algebraic manipulation required to calculate the first 8 terms in the series in (11) (fourteenth order in the WKB approximation) for potentials of the form x^N $(N=2,4,6,\ldots)$.

For potentials of this type the WKB series is a power series in inverse fractional powers of the energy E:

$$E^{1/N+1/2}\sum_{n=0}^{\infty}E^{-n(1+2/N)}\,a_n(N)=(K+\tfrac{1}{2})\pi\,. \tag{12}$$

The coefficients $a_n(N)$ have the form

$$a_n(N)=\frac{2\sqrt{\pi}\,\Gamma\left(1+\dfrac{1-2n}{N}\right)P_n(N)(-1)^n}{\Gamma\left(\dfrac{3-2n}{2}+\dfrac{1-2n}{N}\right)(2n+2)!\,2^n}\,, \tag{13}$$

where P_n is a polynomial in N,[6]

$$\begin{aligned}
P_0(N)&=1\,,\\
P_1(N)&=2(N-1)\,,\\
P_2(N)&=(N-3)(N-1)(2N+3)\,,\\
P_3(N)&=\tfrac{4}{9}(N-5)(N-1)(24N^3+22N^2-117N-139)\,,\\
P_4(N)&=\tfrac{1}{3}(N-7)(N-1)(432N^5-300N^4-5188N^3-1621N^2+14\,716N+12\,961)\,,\\
P_5(N)&=6(N-9)(N-3)(2N+3)(N-1)(320N^5-504N^4-4854N^3-957N^2+14\,754N+12\,801)\,,\\
P_6(N)&=\tfrac{1}{135}(N-11)(N-1)(23\,880\,960N^9-143\,847\,648N^8-391\,498\,152N^7+2\,300\,894\,324N^6+4\,139\,622\,570N^5\\
&\qquad-12\,063\,604\,311N^4-24\,906\,119\,028N^3+13\,770\,853\,986N^2+52\,667\,115\,570N\\
&\qquad+28\,170\,205\,729)\,,\\
P_7(N)&=\tfrac{8}{27}(N-13)(N-1)(43\,545\,600N^{11}-409\,622\,400N^{10}-235\,446\,336N^9+8\,531\,855\,304N^8\\
&\qquad+556\,874\,876N^7-75\,928\,001\,542N^6-38\,662\,114\,659N^5+312\,721\,638\,339N^4\\
&\qquad+352\,177\,852\,074N^3-388\,900\,443\,708N^2-811\,902\,666\,755N-356\,911\,390\,793)\,.
\end{aligned}$$

The formula in (13) immediately explains why it is that the lowest-order WKB approximation in (2) is exact for the harmonic oscillator. If we take $V(x)=x^2$ and thus let $N=2$ in (13) we see that $a_n(2)=0$ when $n\geqslant 1$ because the denominator in (13) is infinite. Thus the series in (12) truncates after the first term.

There is an immediate numerical check of the result in (13). If we take $N=4$ then the series in (12) should give the eigenvalues for the x^4 potential. This series is explicitly

$$E^{3/4}\sum_{n=0}^{\infty}E^{-3n/2}a_n(4)=(K+\tfrac{1}{2})\pi\,, \tag{14}$$

where

$$a_0(4)=\tfrac{1}{3}R\sqrt{\pi}\approx 1.748\,,$$

$$a_1(4)=-\frac{1}{4}\,\frac{\sqrt{\pi}}{R}\approx -0.1498\,,$$

$$a_2(4)=\frac{11}{3\times 2^9}\,R\sqrt{\pi}\approx 0.037\,56\,,$$

$$a_3(4)=\frac{7\times 11\times 61}{3\times 5\times 2^{11}}\,\frac{\sqrt{\pi}}{R}\approx 0.091\,60\,,$$

$$a_4(4)=\frac{5\times 13\times 17\times 353}{7\times 2^{19}}\,R\sqrt{\pi}\approx -0.5574\,,$$

$$a_5(4)=\frac{-11\times 11\times 19\times 23\times 1009}{3\times 2^{21}}\,\frac{\sqrt{\pi}}{R}\approx -5.080\,,$$

$$a_6(4)=\frac{5\times 17\times 29\times 49\,707\,277}{3\times 11\times 2^{28}}\,R\sqrt{\pi}\approx 72.54\,,$$

$$a_7(4)=\frac{3^4\times 7\times 19\times 23\times 31^2\times 109\times 1429}{13\times 2^{30}}\,\frac{\sqrt{\pi}}{R}\approx 1592\,,$$

in which

$$R = \Gamma(\tfrac{1}{4})/\Gamma(\tfrac{3}{4})$$
$$\approx 2.958\,675\,119\,188\,638\,892\,310\,821\,4\,.$$

We have not been able to discover a simple formula for the terms in this series, but the series certainly looks like a typical asymptotic series. Like the Stirling series for the Γ function, the coefficients get smaller for a while but eventually appear to grow without bound. We would therefore expect that for any given value of K, successive approximations to $E^{(K)}$, [obtained by solving (14) with the series truncated after more and more terms] should improve to some maximal accuracy and then become worse. Moreover, since E increases with K, more terms in the series should be required to reach maximal accuracy as K increases and the accuracy should also increase with K. This is precisely what happens for the x^4 potential (see Table I). The rate at which the accuracy increases is particularly impressive.

We do not know if there is a simple generating function for the polynomials $P_n(N)$. However, we have discovered that these polynomials exhibit many startling numerological properties. For example, the real parts of the roots of the polynomials $P_n(N)$ all appear to lie between -2 and $2n-1$. We list below the nth polynomial followed by its roots:

$P_1(N)$: 1.0000;

$P_2(N)$: $-1.5000, 1.0000, 3.0000$;

$P_3(N)$: $-1.8658, -1.3501, 1.0000, 2.2992, 5.0000$;

$P_4(N)$: $-1.9731, -1.5765, -1.3214, 1.0000, 2.1160, 3.4494, 7.0000$;

$P_5(N)$: $-1.9966, -1.6413, -1.5000, -1.3272, 1.0000, 2.0473, 3.0000, 4.4928, 9.0000$;

$P_6(N)$: $-1.9997, -1.6920, -1.4956 \pm 0.1013i, -1.3363, 1.0000, 2.0188, 2.8338, 3.6906, 5.4994, 11.0000$;

$P_7(N)$: $-1.999\,98, -1.7333, -1.5427, -1.4688 \pm 0.1778i, -1.3346,$
$1.0000, 2.0071, 2.8047, 3.3059, 4.3371, 6.499\,98, 13.0000$.

TABLE I. Comparison of the exact eigenvalues of the x^4 potential with the 0, 2, 4, 6, 8, 10, and 12th order WKB predictions from (14). Observe how rapidly the maximal accuracy increases with K.

$E^{(0)}$(exact) ≈ 1.060 362 090 484 182 899 65			$E^{(6)}$(exact) ≈ 26.528 471 883 682 518 191 81		
$(\mathrm{WKB})_0$	0.87		$(\mathrm{WKB})_0$	26.506 335 511	
$(\mathrm{WKB})_2$	0.98	(1 part in 10)	$(\mathrm{WKB})_2$	26.528 512 552	
$(\mathrm{WKB})_4$	0.95		$(\mathrm{WKB})_4$	26.528 471 873	(4 parts in 10^{11})
$(\mathrm{WKB})_6$	0.78		$(\mathrm{WKB})_6$	26.528 471 147	
$(\mathrm{WKB})_8$	1.13		$(\mathrm{WKB})_8$	26.528 471 179	
$(\mathrm{WKB})_{10}$	1.40		$(\mathrm{WKB})_{10}$	26.528 471 182	
$(\mathrm{WKB})_{12}$	1.64		$(\mathrm{WKB})_{12}$	26.528 471 181	
$E^{(2)}$(exact) ≈ 7.455 697 937 986 738 392 16			$E^{(8)}$(exact) ≈ 37.923 001 027 033 985 146 52		
$(\mathrm{WKB})_0$	7.4140		$(\mathrm{WKB})_0$	37.904 471 845 068	
$(\mathrm{WKB})_2$	7.4558	(1 part in 10^5)	$(\mathrm{WKB})_2$	37.923 021 140 528	
$(\mathrm{WKB})_4$	7.4553		$(\mathrm{WKB})_4$	37.923 001 229 358	
$(\mathrm{WKB})_6$	7.4552		$(\mathrm{WKB})_6$	37.923 001 021 414	
$(\mathrm{WKB})_8$	7.4552		$(\mathrm{WKB})_8$	37.923 001 026 832	
$(\mathrm{WKB})_{10}$	7.4552		$(\mathrm{WKB})_{10}$	37.923 001 027 043	(7 parts in 10^{14})
$(\mathrm{WKB})_{12}$	7.4552		$(\mathrm{WKB})_{12}$	37.923 001 027 030	
$E^{(4)}$(exact) ≈ 16.261 826 018 850 225 937 89			$E^{(10)}$(exact) ≈ 50.256 254 516 682 919 039 74		
$(\mathrm{WKB})_0$	16.233 614 7		$(\mathrm{WKB})_0$	50.240 152 319 172 36	
$(\mathrm{WKB})_2$	16.261 936 7		$(\mathrm{WKB})_2$	50.256 265 932 002 07	
$(\mathrm{WKB})_4$	16.261 828 6	(5 parts in 10^8)	$(\mathrm{WKB})_4$	50.256 254 592 948 49	
$(\mathrm{WKB})_6$	16.261 824 5		$(\mathrm{WKB})_6$	50.256 254 515 324 64	
$(\mathrm{WKB})_8$	16.261 824 9		$(\mathrm{WKB})_8$	50.256 254 516 650 43	
$(\mathrm{WKB})_{10}$	16.261 825 0		$(\mathrm{WKB})_{10}$	50.256 254 516 684 34	
$(\mathrm{WKB})_{12}$	16.261 825 0		$(\mathrm{WKB})_{12}$	50.256 254 516 682 99	(1 part in 10^{15})

A cursory observation of these roots leads one to believe that many of the roots lie in sequences. For example, there is a sequence of roots approaching -2 as n, the degree of the polynomials, approaches ∞. There is another sequence which approaches 2, another which approaches $n-\frac{1}{2}$, and possibly one which approaches $(2n-1)/3$.

These observations led us to seek formulas for $P_n(N)$ for these and other special values of N. By trial and error we have discovered the following formulas:

$$P_n(-2)=\frac{-(n+1)(2n+1)!!}{(2n-1)}\ ,$$

$$P_n(n-\tfrac{1}{2})=\frac{-(n+1)[(2n)!]^2}{8^n n!\,(2n-1)}\ ,$$

$$\frac{d}{dx}\,P_n(x)\bigg|_{x=1}=\frac{(-1)^{n+1}(n+1)(2n-2)!\,(2n+1)!!}{3^n}\qquad (n\geq 1)\,,$$

$$P_n(2)=\frac{2(n+1)B_{2n}(2n+1)!!\,(2^{2n-1}-1)}{2n-1}\ ,$$

$$P_n(-1)=\frac{-4^n(2n+1)!!\,(n+1)B_{2n}}{2n-1}\ ,$$

$$P_n(-\tfrac{1}{2})=\frac{-(n+1)(2n+1)(4n-1)(4n+1)(6n+1)!!\,B_{2n}}{(2n-1)(6n-1)(6n+1)(4n+1)!!}\ ,$$

$$P_n\left(\frac{2n-1}{3}\right)=\frac{3(-2)^n n!\,\Gamma((4n+4)/3)}{(2n+3)\Gamma((4-2n)/3)}\ ,$$

$$\text{coefficient of } N^{2n-1} \text{ in } P_n(N)=(n+1)(2n+1)B_{2n}2^n(n-1)!\,(-1)^{n+1}\quad (n\geq 1)\ .$$

In the above formulas B_{2n} is the $2n$th Bernoulli number.[7] The even-numbered Bernoulli numbers $B_0, B_2, B_4, \ldots, B_{14}$ have the values $1, \frac{1}{6}, -\frac{1}{30}, \frac{1}{42}, -\frac{1}{30}, \frac{5}{66}, -\frac{691}{2730}, \frac{7}{6}$. There seems to be a rather deep connection between the polynomials $P_n(N)$ and the Bernoulli polynomials $B_{2n}(x)$.

We hope that the above observations may eventually lead to a better understanding of and possibly a means of generating the polynomials $P_n(N)$.

B. Exactly soluble potentials

There are several well-known potentials whose eigenvalues can be determined in closed form. Besides the harmonic oscillator, there are the potentials

$$V(x)=-\frac{V_0}{\cosh^2 x}\qquad\text{and}\qquad V(x)=Ae^{-2ax}-Be^{-ax}\ . \tag{15}$$

These potentials are discussed by Rosenzweig and Krieger (see Ref. 2).

We examined the WKB series in (11) for the potential in (15). We found that for this potential the WKB series reduces to a geometric series which can be summed to give the exact energy eigenvalues. We summarize our analysis very briefly.

We first verify by induction that a solution to (6) for $V(x)$ in (15) has the general form

$$S_n'=(S_0')^{1-3n}P_n(\operatorname{sech} z)\times\begin{cases}1, & n \text{ even}\\ \sinh z, & n \text{ odd}\,,\end{cases}$$

where P_n is a polynomial of the form

$$P_n(u)=A_{n,0}u^{3n}+A_{n,1}u^{3n-2}+\cdots+\begin{cases}A_{n,(3n/2-1)}u^2, & n\text{ even}\\ A_{n,(3n/2-3/2)}\,u^3, & n\text{ odd}\,.\end{cases}$$

The integrals in (11) are performed by substituting $w=\sinh z$. The nth term in (11) reduces to

$$\sum_{l=0}^{3n-1}A_{2n,l}\,\frac{1}{2i}\oint\frac{(1+w^2)^{l-1}dw}{(-V_0-E-Ew^2)^{(6n-1)/2}}=\begin{cases}\pi\sqrt{V_0}-\pi\sqrt{-E}\,, & n=0\\ \pi A_{2n,0}\sqrt{V_0}\,(-V_0{}^3)^n, & n>0\,.\end{cases}$$

Thus, we need only find the coefficient $A_{2n,0}$ explicitly.

The recursion relation for $A_{n,0}$ is

$$A_{n,0}=\tfrac{1}{2}\left(V_0A_{n-1,0}-\sum_{i=1}^{n-1}A_{i,0}A_{n-i,0}\right), \quad A_{0,0}=1,$$

whose solution is

$$A_{2n,0}=(-1)^n(V_0/2)^{2n}\binom{\frac{1}{2}}{n},$$

$$A_{1,0}=V_0/2,$$

$$A_{2n+3,0}=0.$$

The quantization condition in (11) thus becomes

$$\pi\sum_{n=0}^{\infty}\sqrt{V_0}\binom{\frac{1}{2}}{n}\left(\frac{1}{4V_0}\right)^n-\pi\sqrt{-E}=\pi(V_0+\tfrac{1}{4})^{1/2}-\pi\sqrt{-E}$$

$$=(K+\tfrac{1}{2})\pi.$$

Hence, solving for E gives

$$E=-(V_0+\tfrac{1}{4})^{1/2}-(K+\tfrac{1}{2})^2, \tag{17}$$

where $0\leq K\leq(V_0+\frac{1}{4})^{1/2}-\frac{1}{2}$. The result in (17) is exact.

III. GENERAL EXAMINATION OF S'_{2n} FOR ARBITRARY POTENTIALS

In this section we catalog the properties of S'_n for arbitrary n. We have already listed S'_0, S'_1, S'_2, and S'_3 in (5), (7), (8), and (9). It is clear that the number of terms in S'_n grows rapidly with n. In fact, the number of terms in S'_n is exactly equal to $p(n)$, the number of partitions of n (see Table II).

Given S'_n we can construct various elements in the equivalence class E_n by adding total derivatives. These derivatives are constructed by taking the terms in $S'_{n-1}(x)$, one at a time, multiplying each by $1/\sqrt{Q}$, and differentiating with respect to x. This gives $p(n-1)$ individual total derivatives which may be added or subtracted from $S'_n(x)$. For example, to $S'_4(x)$ we can add arbitrary quantities of

$$\frac{d}{dx}\left[\frac{Q'''(x)}{Q^{5/2}}\right],\quad \frac{d}{dx}\left[\frac{Q'(x)Q''(x)}{Q^{7/2}}\right],\quad \frac{d}{dx}\left\{\frac{[Q'(x)]^3}{Q^{9/2}}\right\}.$$

TABLE II. Number of partitions $p(n)$ for $n=0,1,2,\ldots,12$. The number of terms in S'_n is $p(n)$.

n	$p(n)$
0	1
1	1
2	2
3	3
4	5
5	7
6	11
7	15
8	22
9	30
10	42
11	56
12	77

TABLE III. Three elements of E_4. Notice how simple T'_4 and U'_4 are compared with S'_4.

Structure of term	Coefficient for S'_4	Coefficient for T'_4	Coefficient for U'_4
$\frac{Q''''}{Q^{5/2}}$	$-\frac{1}{32}$	$\frac{-\Gamma(\frac{5}{2})}{2\times 2!\,12^2\Gamma(\frac{1}{2})}$	0
$\frac{Q'Q''}{Q^{7/2}}$	$\frac{7}{32}$	0	0
$\frac{Q''^2}{Q^{7/2}}$	$\frac{19}{128}$	$\frac{7}{1536}$	$4^{-2-3/2}$
$\frac{Q'^2Q''}{Q^{9/2}}$	$-\frac{221}{256}$	0	$\frac{-\Gamma(\frac{9}{2})}{2\times 2!\,3^24^2\Gamma(\frac{1}{2})}$
$\frac{Q'^4}{Q^{11/2}}$	$\frac{1105}{2048}$	0	0

TABLE IV. Three elements of E_6. In U'_6 the number α is an arbitrary parameter.

Structure of term	Coefficient for S'_6	Coefficient for T'_6	Coefficient for U'_6
$\frac{Q''''''}{Q^{7/2}}$	$-\frac{1}{128}$	$\frac{-\Gamma(\frac{7}{2})}{2\times 3!\,12^3\Gamma(\frac{1}{2})}$	0
$\frac{Q'Q'''''}{Q^{9/2}}$	$\frac{27}{256}$	0	0
$\frac{Q''Q''''}{Q^{9/2}}$	$\frac{55}{256}$	$\frac{7}{4096}$	$4^{-3-3/2}$
$\frac{Q'''^2}{Q^{9/2}}$	$\frac{69}{512}$	$\frac{1}{13824}$	0
$\frac{Q'^2Q''''}{Q^{11/2}}$	$-\frac{315}{1024}$	0	0
$\frac{Q'Q''Q'''}{Q^{11/2}}$	$-\frac{1391}{512}$	0	$\frac{12-\alpha}{2^{10}}$
$\frac{Q''^3}{Q^{11/2}}$	$-\frac{631}{1024}$	$-\frac{31}{8192}$	$\frac{1-\alpha}{2^{11}}$
$\frac{Q'^3Q'''}{Q^{13/2}}$	$\frac{1055}{256}$	0	0
$\frac{Q'^2Q''^2}{Q^{13/2}}$	$\frac{34\,503}{4096}$	0	$\frac{11\alpha}{2^{12}}$
$\frac{Q'^4Q''}{Q^{15/2}}$	$-\frac{248\,475}{16\,384}$	0	$\frac{-\Gamma(\frac{15}{2})}{2\times 3!\,12^3\Gamma(\frac{1}{2})}$
$\frac{Q'^6}{Q^{17/2}}$	$\frac{414\,125}{65\,536}$	0	0

TABLE V. Three elements of E_8. U_8' is a four-parameter class in which α, β, γ, and δ are arbitrary numbers.

Structure of term	Coefficient for S_8'	Coefficient for T_8'	Coefficient for U_8'
$Q''''''''Q^{-9/2}$	$-\frac{1}{512}$	$\frac{-\Gamma(\frac{9}{2})}{2\times 4!\,12^4\Gamma(\frac{1}{2})}$	0
$Q'Q'''''''Q^{-11/2}$	$\frac{11}{256}$	0	0
$Q''Q''''''Q^{-11/2}$	$\frac{119}{1024}$	$\frac{77}{294\,912}$	$4^{-4-3/2}$
$Q'''Q'''''Q^{-11/2}$	$\frac{209}{1024}$	$\frac{1}{184\,32}$	0
$Q''''^2Q^{-11/2}$	$\frac{251}{2048}$	$\frac{33}{131\,072}$	0
$Q'^2Q''''''Q^{-13/2}$	$-\frac{2135}{4096}$	0	0
$Q'Q''Q'''''Q^{-13/2}$	$-\frac{2547}{1024}$	0	$\frac{3503}{2^{11}}-2\alpha$
$Q'Q'''Q''''Q^{-13/2}$	$-\frac{3847}{1024}$	0	0
$Q''^2Q''''Q^{-13/2}$	$-\frac{10\,461}{4096}$	$-\frac{2717}{655\,360}$	$\frac{1083}{2^{11}}-2\alpha+\beta$
$Q''Q'''^2Q^{-13/2}$	$-\frac{13\,161}{4096}$	$-\frac{121}{368\,640}$	$\frac{-13\,161}{2^{12}}+\alpha+2\beta$
$Q'^3Q'''''Q^{-15/2}$	$\frac{36\,195}{8192}$	0	0
$Q'^2Q''Q''''Q^{-15/2}$	$\frac{223\,431}{8192}$	0	$\frac{-273\,277}{2^{14}}+\frac{39}{2}\alpha$
$Q'^2Q'''^2Q^{-15/2}$	$\frac{281\,237}{16\,384}$	0	0
$Q'Q''^2Q'''Q^{-15/2}$	$\frac{47\,919}{1024}$	0	$\frac{102\,115}{2^{13}}+13\alpha-\frac{13\beta}{2}+3\gamma$
$Q''^4Q^{-15/2}$	$\frac{174\,317}{32\,768}$	$\frac{18\,161}{2\,621\,440}$	$\frac{174\,317}{2^{15}}+\gamma$
$Q'^4Q''''Q^{-17/2}$	$-\frac{1\,841\,055}{65\,536}$	0	0
$Q'^3Q''Q'''Q^{-17/2}$	$-\frac{3\,164\,229}{16\,384}$	0	$\frac{-641\,793}{2^{15}}-\frac{13\times 15}{4}\alpha+2\delta$
$Q'^2Q''^3Q^{-17/2}$	$-\frac{4\,321\,753}{32\,768}$	0	$\frac{-4\,321\,753}{2^{15}}-\frac{15}{2}\gamma+3\delta$
$Q'^5Q'''Q^{-19/2}$	$\frac{8\,905\,935}{65\,536}$	0	0
$Q'^4Q''^2Q^{-19/2}$	$\frac{121\,782\,417}{262\,144}$	0	$\frac{17\times 4\,026\,651}{2^{18}}-\frac{17}{2}\delta$
$Q'^6Q''Q^{-21/2}$	$-\frac{256\,406\,305}{524\,288}$	0	$\frac{-\Gamma(\frac{21}{2})}{2\times 4!\,12^4\Gamma(\frac{1}{2})}$
$Q'^8Q^{-23/2}$	$\frac{1\,282\,031\,525}{8\,388\,608}$	0	0

TABLE VI. Comparison of T'_{2n} for various values of p. $A(x)$ and $Q(x)$ are related by $Q=A^{2p}$. When $p=\frac{1}{2}$ we recover the coefficients for T'_{2n} listed in Tables III–V. By contrast, when $p=-\frac{2}{3}$, the numerators of the coefficients are all 1 and the denominators are all powers of 2, 3, and 5. We do not understand why this simplification occurs.

Structure of term	Coefficient for $p=\frac{1}{2}$	Coefficient for $p=-\frac{2}{3}$	Coefficient for arbitrary p
		Second-order WKB	
$\frac{A''}{A^{p+1}}$	$\frac{-\Gamma(\frac{3}{2})}{2\times 1!12\Gamma(\frac{1}{2})}$	$-\frac{1}{2\times 3}$	$\frac{-p^2}{2^3(p+1)}$
		Fourth-order WKB	
$\frac{A''''}{A^{3p+1}}$	$\frac{-\Gamma(\frac{5}{2})}{2\cdot 2!12^2\Gamma(\frac{1}{2})}$	0 [a]	$\frac{-p^2(p+2)}{2^7(p+1)(3p+1)}$
$\frac{A''^2}{A^{3p+2}}$	$\frac{7}{1536}$	$\frac{1}{2^3 3^2}$ [a]	$\frac{p^2(3p+2)}{2^7(p+1)}$
		Sixth-order WKB	
$\frac{A''''''}{A^{5p+1}}$	$\frac{-\Gamma(\frac{7}{2})}{2\times 3!12^3\Gamma(\frac{1}{2})}$	0	$\frac{-p^2(p+2)(3p+2)(3p+4)}{2^{10}(p+1)(5p+1)(5p+2)(5p+3)}$
$\frac{A'''^2}{A^{5p+2}}$	$\frac{1}{13\,824}$	$\frac{-1}{2^5 3^2}$	$\frac{-p^2(28p^3+20p^2-12p-8)}{2^9(p+1)(5p+2)(5p+3)}$
$\frac{A''A''''}{A^{5p+2}}$	$\frac{7}{4096}$	0	$\frac{3(3p+2)(3p+4)p^2}{2^{10}(p+1)(5p+3)}$
$\frac{A''^3}{A^{5p+3}}$	$\frac{-31}{2^{13}}$	$\frac{-1}{2^5 3^3}$	$\frac{-p^2(79p^3+160p^2+108p+24)}{2^{10}(p+1)(5p+3)}$
		Eighth-order WKB	
$\frac{A''''''''}{A^{7p+1}}$	$\frac{-\Gamma(\frac{9}{2})}{2\times 4!12^4\Gamma(\frac{1}{2})}$	0	$\frac{-5p^2(p+2)(3p+2)(3p+4)(5p+4)(5p+6)}{2^{15}(p+1)(7p+5)(7p+4)(7p+3)(7p+2)(7p+1)}$
$\frac{A''A''''''}{A^{7p+2}}$	$\frac{77}{294\,912}$	0	$\frac{5p^2(3p+2)(3p+4)(5p+4)(5p+6)}{2^{13}(p+1)(7p+5)(7p+4)(7p+3)}$
$\frac{A'''A'''''}{A^{7p+2}}$	$\frac{1}{18\,432}$	$\frac{-1}{2^7 3^2 5}$	$\frac{-p^2(5p+4)(187p^4+281p^3-130p-40)}{2^9(p+1)(7p+5)(7p+4)(7p+3)(7p+2)}$
$\frac{A''''^2}{A^{7p+2}}$	$\frac{33}{131\,072}$	$\frac{1}{2^5 3^2 5}$	$\frac{p^2(61\,199p^5+181\,450p^4+222\,548p^3+147\,064p^2+53\,312p+8320)}{2^{15}(p+1)(7p+5)(7p+4)(7p+3)(7p+2)}$
$\frac{A''^2A''''}{A^{7p+3}}$	$-\frac{2717}{655\,360}$	$\frac{-1}{2^7 3^2 5}$	$\frac{-3p^2(5p+4)(4883p^4+13\,346p^3+12\,908p^2+5320p+800)}{2^{14}(p+1)(7p+5)((7p+4)(7p+3)}$
$\frac{A''A'''^2}{A^{7p+3}}$	$-\frac{121}{368\,640}$	$\frac{1}{2^4 3^3 5}$	$\frac{p^2(2453p^5+4957p^4+2091p^3-1630p^2-1512p-320)}{2^{10}(p+1)(7p+5)(7p+4)(7p+3)}$
$\frac{A''^4}{A^{7p+4}}$	$\frac{18\,161}{2\,621\,440}$	$\frac{1}{2^7 3^4}$	$\frac{p^2(33\,997p^5+121\,062p^4+171\,404p^3+120\,360p^2+41\,856p+5760)}{2^{15}(p+1)(7p+5)(7p+4)}$

[a] Note that by adding total derivatives the positions of 0 and $2^{-3}3^{-2}$ may be reversed.

What is the best strategy for simplifying $S'_{2n}(x)$? One approach is to argue that since there are precisely $p(n-1)$ terms in $S'_n(x)$ which contain $Q'(x)$, we can eliminate just these terms using the $p(n-1)$ total derivatives at our disposal. The resulting elements of E_{2n}, which we call T'_{2n}, have many fewer terms and their numerical coefficients are much simpler than those of S'_n (see Tables III–V). The marked simplification in the coefficients that occurs when we transform from S'_{2n} to T'_{2n} holds without exception up through twelfth order in the WKB approximation. This is one of many unexplained numerological observations. We have also observed that the coefficient of the $Q^{2n}Q^{-n-1/2}$ term in T'_{2n} has the general form $-\Gamma(n+\frac{1}{2})/[2\times n!\,12^n\Gamma(\frac{1}{2})]$ and that the coefficient of $Q''^nQ^{-2n+1/2}$ has the general form $(2^{1-2n}-1)B_{2n}(4n-3)!!/(2n)!$.

Another approach is to eliminate all terms from S'_n which do not contain $Q''(x)$. Since this can be achieved using fewer than the $p(n-1)$ total derivatives, the result, which we call $U'_n(x)$, contains arbitrary parameters when $n>4$. For special choices of these parameters the numerical coefficients can be made extremely simple (see Tables III–V). We have observed that in U'_{2n} the coefficient of the $Q''Q^{2n-2}Q^{-n-3/2}$ term has the general form

$$4^{-n-3/2}$$

and the coefficient of the $Q''Q'^{2n-2}Q^{-3n+3/2}$ has the general form

$$-\Gamma(3n-\tfrac{3}{2})/[2\times n!\,12^n\Gamma(\tfrac{1}{2})]\,.$$

There are a number of other approaches one can use to try to simplify the elements of S'_n. For example, one may rewrite S'_n in terms of $A(x)$, which is related to $Q(x)$ by

$$Q=A^{2p},$$

where p is a number. Once $S'_n(x)$ is written in terms of $A(x)$, the result may be simplified to T-type structures, in which no $A'(x)$ terms appear, or U-type structures, in which all terms contain $A''(x)$. We have found that there are special choices for p which make the resulting structures extremely simple. However, once again we cannot provide any explanation for these numerological facts. (See Table VI.)

We do not know whether the simplification in the coefficients in Table VI that occurs when $p=-\frac{2}{3}$ persists in higher order or if there is a sequence of p's (one for each order) which simplifies the coefficients in nth order in a predictable way. Also, it may be useful to try a U-type reduction and then search for values of p which give simple results.

We have carried out many further numerological experiments up to twelfth order in the WKB approximation which we will not present here. The one common conclusion of these experiments is that for some unknown reason the elements of E_{2n} are trying to be simple. We do not yet have a prescription for achieving maximal simplicity and we certainly do not know whether it will be possible to actually guess a formula for the simplest element of E_{2n}. However, we hope we have succeeded in presenting a convincing argument that there is at least a possibility that the rich structure of the recursion relation in (6) may eventually be understood.

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[1]J. L. Dunham, Phys. Rev. 41, 713 (1932).

[2]This result was known to C. Rosenzweig and J. B. Krieger, J. Math. Phys. 9, 849 (1968).

[3]To understand why $S'_{2n+1}(x)$ $(n\geq 1)$ is a total derivative, we note that the quantization condition in (10) is a constraint on the phase of y. $S'_{2n+1}(x)$ $(n\geq 1)$ is always *real* because it contains no fractional powers of $V-E$ and therefore cannot contribute to the *phase* of $y(x)$. It is $S'_{2n}(x)$ which becomes imaginary as x crosses into a classically allowed region and causes the wave function to become oscillatory. It is then no surprise that S'_{2n+1} drops out of the quantization condition.

[4]In general, for the Nth-order equation

$$\epsilon^N\frac{d^N}{dx^N}\,y(x)=Q(x)y(x)\,,$$

substituting

$$y(x)=\frac{1}{\epsilon}\sum_{n=0}^{\infty}\epsilon^n S_n(x)$$

gives a nonlinear recursion relation for $S'_n(x)$. We find that every Nth $S'_n(x)$ is a total derivative, starting with $S'_{N+1}(x)$, $S'_{2N+1}(x)$, $S'_{3N+1}(x)$, ...

[5]V. Zakharov and L. Faddeev, Funct. Anal. Appl. 5, 280 (1972).

[6]We thank J. A. Paget for computing $P_7(N)$.

[7]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun, National Bureau of Standards, Applied Mathematics Series, No. 55 (U.S. G.P.O., Washington, D.C., 1970), p. 804.