

# Improving the accuracy of WKB eigenvalues

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A simple method is proposed for improving the accuracy of WKB eigenvalues by using the WKB eigenfunctions as trial functions in a variational-principle expression for the eigenvalues. The first-order eigenvalues obtained from this estimate are shown to differ from the exact values by terms of order  $\epsilon^6$  (where  $\epsilon$  is an appropriately defined small parameter that specifies the accuracy of the WKB approximation). For comparison, the fifth-order WKB eigenvalues also differ from the exact values by terms of order  $\epsilon^6$ . Higher-order variational eigenvalues are also defined, and the third-order estimate is shown to differ from the exact by terms of order  $\epsilon^{10}$ . The accuracy of these variational and WKB estimates are illustrated with a numerical example.

## I. INTRODUCTION

We consider the problem of estimating the eigenvalues of the differential equation,

$$y'' + \kappa f(x)y = 0, \quad (1)$$

having the boundary conditions  $y(0) = y(l) = 0$ . The given function  $f$  is assumed to be smooth and positive on  $[0, l]$ ; and prime represents differentiation with respect to  $x$ . We estimate the eigenvalue of the  $n$ th mode of this equation to be

$$\kappa_n \approx \left(\frac{\pi}{L}\right)^2 \left(n^2 + \frac{2}{\pi} \int_0^l v[\varphi(x)] \sin^2[n\varphi(x)] \frac{d\varphi}{dx} dx\right), \quad (2)$$

where the function  $\varphi(x)$  is given by

$$\varphi(x) = \frac{\pi}{L} \int_0^x f^{1/2}(\xi) d\xi, \quad (3)$$

$v[\varphi(x)]$  is defined by

$$v[\varphi(x)] = f^{-1/4} \frac{d^2 f^{1/4}}{d\varphi^2} = \frac{L^2 [4ff'' - 5(f')^2]}{16\pi^2 f^3}, \quad (4)$$

and  $L$  is the integral given by

$$L = \int_0^l f^{1/2}(x) dx. \quad (5)$$

In this paper we derive this estimate from a variational-principle expression for the eigenvalue. We evaluate the accuracy of this estimate and show that it is accurate to order  $\epsilon^6$  in terms of an appropriate WKB smallness parameter  $\epsilon$  to be defined later. The first term on the right side of Eq. (2),  $(n\pi/L)^2$ , is the standard first-order WKB eigenvalue which, for comparison, is accurate to order  $\epsilon^2$ . The accuracy of the WKB eigenvalues can be considerably improved, therefore, with very little additional effort. In Sec. II we derive this estimate for the eigenvalue, and evaluate its accuracy. In Sec. III we consider higher-order WKB (and the analogous phase-integral) approximations for this eigenvalue problem, and compare their accuracy to the estimate derived here. We find that the fifth-order WKB eigenvalues are also accurate to order  $\epsilon^6$ . In Sec. IV we outline how a sequence of higher-order variational estimates of the eigenvalues can be constructed from the higher-order WKB eigenfunctions. We show that the variational estimate based on the third-order

WKB eigenfunction is accurate to order  $\epsilon^{10}$ . Finally, in Sec. V we illustrate the accuracy of these various estimates for a specific numerical example. We find that our estimate is considerably better than the fifth-order WKB estimate for small values of  $n$ , while the fifth-order WKB eigenvalues are more accurate for large values of  $n$ .

## II. THE FIRST-ORDER VARIATIONAL ESTIMATE

One standard technique for estimating the eigenvalues  $\kappa$  of Eq. (1) uses the variational principle:

$$\kappa[y] = \int_0^l (y')^2 dx \left[ \int_0^l f y^2 dx \right]^{-1}. \quad (6)$$

Once an estimate of the eigenfunction  $y$  is found, it is easy to use Eq. (6) to obtain an estimate of the eigenvalue (which will be more accurate than  $y$  itself).<sup>1</sup> When the function  $f(x)$  is sufficiently slowly varying on the interval  $[0, l]$  an alternate approach, the WKB method, is known to produce useful approximations to the eigenvalues and eigenfunctions for this problem. The first-order WKB functions and eigenvalues have the well-known forms:<sup>2</sup>

$$y_n(x) = (2/L)^{1/2} f^{-1/4} \sin(n\varphi), \quad (7)$$

$$\kappa_n = (n\pi/L)^2, \quad (8)$$

where  $\varphi(x)$  and  $L$  are given in Eqs. (3) and (5). It seems natural to consider the possibility of using the WKB functions  $y_n$  as the trial eigenfunctions in the variational principle, Eq. (6), to obtain improved eigenvalues. (We are not aware of their having been used in this way before, however.) We investigate here, analytically and through a numerical example, the accuracy of the eigenvalues obtained in this way.

In order to make the analysis of the accuracy of these approximation techniques more straightforward, it is convenient to transform Eq. (1) into the following equivalent form:

$$\ddot{w} + \lambda w = v(\varphi)w, \quad (9)$$

with the boundary conditions  $w(0) = w(\pi) = 0$ . The independent variable  $x$  has been replaced with the variable  $\varphi$  [with domain  $[0, \pi]$  as defined in Eq. (3)] and the depen-

dent variable  $y$  has been replaced with  $w = f^{1/4}y$ . The “dot” represents differentiation with respect to  $\varphi$ , and the eigenvalue  $\kappa$  has been replaced with its dimensionless counterpart  $\lambda = \kappa(L/\pi)^2$ . It is straightforward to verify that Eq. (9) is equivalent to Eq. (1) when the function  $v$  is defined as in Eq. (4). In this formulation the first-order WKB approximation is almost trivial. If the function  $f$  is suitably “slowly varying” the function  $v$  will be negligible compared to  $\lambda$ . Under these circumstances the functions,

$$w_n(\varphi) = (2/\pi)^{1/2} \sin(n\varphi), \quad (10)$$

(approximately) satisfy Eq. (9) with  $\lambda = n^2$ . The functions  $w_n$  are, then, the first-order WKB eigenfunctions normalized to be orthonormal with respect to integrals over  $\varphi$ . To make the needed “slowly varying” assumption on the function  $f$  precise, we require that

$$|v(\varphi)| \leq \epsilon^2, \quad (11)$$

for some small constant  $\epsilon$ . We have chosen the quadratic dependence on the small constant  $\epsilon$  to be consistent with more conventional formulations of the conditions under which the WKB approximation applies.<sup>2</sup> In order to extend our analysis beyond the simple first-order WKB functions and eigenvalues, we will require in addition that the function  $v$  itself be slowly varying. In particular we require that

$$\left| \frac{d^k v}{d\varphi^k} \right| \leq \epsilon^{k+2}, \quad (12)$$

for  $k = 1, 2$ . The small constant  $\epsilon$  is taken to have the same value as in Eq. (11). These conditions are analogous (but not identical) to the conditions that are imposed on the function  $f$  in order to proceed with higher-order WKB expansions.<sup>2,3</sup> Equations (11) and (12) serve, effectively, as the definition of the parameter  $\epsilon$ . These equations can, for given  $\epsilon$ , be considered as constraints on the potentials  $f(x)$  allowed by our approximation. Alternatively, for a given potential these equations determine the magnitude of the constant  $\epsilon$  and hence the size of the errors in the various approximations that follow.

We begin by using the variational principle to estimate the eigenvalues of Eq. (9) using the WKB functions as test eigenfunctions:

$$\mu_n \equiv \lambda_n[w_n] = \int_0^\pi [(\dot{w}_n)^2 + (w_n)^2 v] d\varphi = n^2 + v_{nn}, \quad (13)$$

where

$$v_{mn} = \int_0^\pi v w_m w_n d\varphi. \quad (14)$$

We note that Eq. (13) is precisely the estimate given in Eq. (2):  $\kappa_n \approx (\pi/L)^2 \mu_n$ . The next step is to obtain sufficiently accurate expressions for the exact eigenvalues  $\lambda_n$  so that the accuracy of the first-order WKB eigenvalues  $n^2$  and the variational eigenvalues  $\mu_n$  may be evaluated. This is easy to accomplish because the exact differential equation (9) has been written in a form that makes it appear to be a small perturbation of the WKB equation (or in this form the harmonic oscillator equation). Thus the value of the exact eigenvalue  $\lambda_n$  may readily be determined to any degree of

accuracy using well-known perturbation theory techniques.<sup>4</sup> The resulting expression for  $\lambda_n$  can be written as

$$\lambda_n = n^2 + v_{nn} + E_n = \mu_n + E_n, \quad (15)$$

where  $E_n$  is the difference between the exact and the variational eigenvalues. Keeping terms through order  $v^2$  in the standard formulas,  $E_n$  is given by

$$E_n = \sum_{m \neq n} \frac{(v_{mn})^2}{n^2 - m^2} + O(v_{ij}^3). \quad (16)$$

Since the  $v_{mn}$  are (nominally) of order  $\epsilon^2$ , we might (naively) conclude from Eqs. (14)–(16) that the variational eigenvalues  $\mu_n$  differ from the exact values by terms of order  $\epsilon^4$ , while the WKB eigenvalues  $n^2$  differ from the exact values by terms of order  $\epsilon^2$ . This conclusion would not be correct, however, for differential equations whose potential  $f$  satisfies Eqs. (11)–(12), because in this case the  $v_{mn}$  for  $m \neq n$  are in fact of order  $\epsilon^3$ .

In order to evaluate the magnitude of  $E_n$  (the difference between the exact and variational eigenvalues) we need a more precise estimate of the magnitude of the  $v_{mn}$ . Using the identity  $(2\pi)^{1/2}(n^2 - m^2)w_n w_m = (n+m)\dot{w}_{n-m} - (n-m)\dot{w}_{n+m}$ , Eq. (14) can be transformed into the following form (when  $n \neq m$ ):

$$v_{mn} = (2\pi)^{-1/2} \int_0^\pi \dot{v} \left( \frac{w_{n+m}}{n+m} - \frac{w_{n-m}}{n-m} \right) d\varphi. \quad (17)$$

We can evaluate this expression (up to terms of order  $\epsilon^4$ ) by using the mean value theorem for derivatives:

$$\dot{v}(\varphi) = \dot{v}(0) + \varphi \ddot{v}[\phi(\varphi)], \quad (18)$$

where  $\phi(\varphi)$  is a function whose range is a subset of its domain  $[0, \pi]$ . Since  $\ddot{v}$  is of order  $\epsilon^4$  by assumption [Eq. (12)], it is straightforward to show that (for  $m \neq n$ )

$$v_{mn} = [(-1)^{m+n} - 1] \frac{4mn\dot{v}(0)}{\pi(m^2 - n^2)^2} + O(\epsilon^4). \quad (19)$$

This expression can now be inserted into Eq. (16) to obtain the desired expression for the error in the variational eigenvalues:

$$E_n = [\dot{v}(0)]^2 \sigma_n / n^2 + O(\epsilon^7), \quad (20)$$

where  $\sigma_n$  is the sum defined by

$$\sigma_n \equiv \sum_{m \neq n} \frac{16n^4 m^2 [1 - (-1)^{m+n}]^2}{\pi^2 (n^2 - m^2)^5} = \frac{\pi^2}{48} - \frac{5}{16n^2}. \quad (21)$$

Equation (20) demonstrates that the variational-principle eigenvalues are accurate to order  $\epsilon^6$  and that the error decreases with increasing mode number as  $n^{-2}$ . The fractional error in the eigenvalue decreases with increasing mode numbers as  $n^{-4}$ . The derivation of the second equality in Eq. (21) is presented in Sec. IV.

### III. HIGHER-ORDER WKB ESTIMATES

The variational estimate of the eigenvalues, Eq. (2), represents a substantial improvement in accuracy over the WKB estimate as we have shown in Sec. II. Of course, other methods exist for improving the accuracy of the WKB eigenvalues. In particular, the higher-order WKB approximation also provide estimates of the eigenvalues of Eq. (1). It is

appropriate, therefore, to compare the accuracy of the eigenvalues obtained by the variational method with those obtained using the higher-order WKB (or equivalently the higher-order phase-integral<sup>5</sup>) approximations. In this section, we derive expressions for the WKB eigenvalues through fifth order and evaluate their accuracy.

The fifth-order phase-integral solution of Eq. (1) that satisfies the boundary condition  $y(0) = 0$  may be written in the form<sup>5</sup>

$$y(x) = q^{-1/2}(x) \sin \left[ \int_0^x q(x') dx' \right], \quad (22)$$

where

$$q(x) = \frac{\pi(\lambda_n f)^{1/2}}{L} \left( 1 - \frac{v}{2\lambda_n} + \frac{\ddot{v} - v^2}{8\lambda_n^2} \right). \quad (23)$$

The constant  $\lambda_n$  that appears in this expression is the dimensionless eigenvalue which is related to the eigenvalue of Eq. (1) by  $\lambda_n = (L/\pi)^2 \kappa_n$ . This function satisfies the second boundary condition,  $y(l) = 0$ , if and only if the argument of the sin function in Eq. (22) has the value  $n\pi$  (for some integer  $n$ ) at  $x = l$ . This condition leads to the following equation for  $\gamma_n^{(5)}$ , the dimensionless form of the fifth-order phase-integral eigenvalue:

$$0 = (\gamma_n^{(5)})^2 - n(\gamma_n^{(5)})^{3/2} - A^{(3)}\gamma_n^{(5)} - A^{(5)}, \quad (24)$$

where the coefficients  $A^{(3)}$  and  $A^{(5)}$  are defined by

$$A^{(3)} = \frac{1}{2\pi} \int_0^\pi v d\varphi, \quad (25)$$

and

$$A^{(5)} = \frac{1}{8\pi} \int_0^\pi (v^2 - \ddot{v}) d\varphi. \quad (26)$$

The fifth-order WKB solutions to Eq. (1) are proportional to the fifth-order phase-integral solution, Eq. (22). Since the function of proportionality is nonvanishing, it follows that the fifth-order WKB eigenvalues also satisfy Eq. (24). We also note that the third-order WKB (or phase-integral) estimates for the eigenvalues are roots of Eq. (24) when  $A^{(5)}$  is set to zero.

The fifth-order WKB estimate for the eigenvalue  $\gamma_n^{(5)}$  is the root of Eq. (24) that reduces to  $n^2$  when  $A^{(3)}$  and  $A^{(5)}$  are set to zero. It is relatively straightforward to solve this equation to sufficiently high order in powers of  $\epsilon$  when  $v$  and its derivatives satisfy the slow variation conditions [Eqs. (11)–(12)] for  $k = 1, 2, 3, 4, 5$ . Note that these are stronger conditions than were needed to evaluate the variational estimate to the same order. Using the mean-value theorem [Eq. (18)], simple trigonometric identities, and performing numerous integrations by parts, it follows that  $\gamma_n^{(5)}$  is related to the exact (dimensionless) eigenvalue  $\lambda_n$  [whose value is given to this order in Eqs. (15), (20)–(21)] by

$$\gamma_n^{(5)} = \lambda_n - \Delta_n^{(5)}, \quad (27)$$

where the error term  $\Delta_n^{(5)}$  is given by

$$\Delta_n^{(5)} = \frac{1}{16n^4} \left[ 2v^3(0) - 5\dot{v}^2(0) - 6v(0)\ddot{v}(0) + \frac{d^4v(0)}{d\varphi^4} \right] + O(\epsilon^7). \quad (28)$$

For comparison, the analogous error term for the third-order WKB eigenvalue  $\gamma_n^{(3)}$  is given by

$$\Delta_n^{(3)} = [v^2(0) - \ddot{v}(0)]/4n^2 + O(\epsilon^5). \quad (29)$$

It is easy to see that the error  $E_n$  [from Eq. (20)] for the variational-eigenvalue estimate is smaller by a factor of order  $\epsilon^2$  than the third-order WKB error  $\Delta_n^{(3)}$  [from Eq. (29)]. Each of these errors varies with mode number as  $n^{-2}$ . Thus the variational estimate is expected to be more accurate than the third-order WKB estimate for all values of  $n$ . The error term  $E_n$  is of the same order in  $\epsilon$  as the fifth-order WKB error  $\Delta_n^{(5)}$  [from Eq. (28)], and thus might be expected to be of roughly comparable accuracy. However, since  $E_n$  varies with mode number as  $n^{-2}$  while  $\Delta_n^{(5)}$  varies as  $n^{-4}$ , the fifth-order WKB estimate will be more accurate for sufficiently large values of  $n$ . In contrast, since  $E_n$  depends only on first derivatives of  $v$  while  $\Delta_n^{(5)}$  depends on its derivatives up to the fourth, it is likely (i.e., for most  $v$ ) that  $E_n$  will be smaller than  $\Delta_n^{(5)}$  for small values of  $n$ .

#### IV. HIGHER-ORDER VARIATIONAL ESTIMATES

Just as the WKB approximation can be extended to a sequence of higher-order approximations, the variational method can also be used to obtain a sequence of higher-order estimates for the eigenvalues of Eq. (1). The natural extension of the first-order variational estimate developed in Sec. II is to use the higher-order WKB eigenfunctions as the trial functions in the variational principle, Eq. (6). In this section we outline how this extension to higher order can be implemented. We explicitly derive a third-order variational estimate for the eigenvalues. As in Sec. II we perform the derivation in such a way that it is straightforward to obtain an expression for the error term. The third-order variational estimate differs from the exact eigenvalue by terms of order  $\epsilon^{10}$ .

As in the first-order variational estimate discussed in Sec. II, it is convenient to introduce new variables that transform the differential equation (1) into a form more suited to the approximation scheme. Thus we introduce as the new independent variable the third-order phase<sup>5</sup>

$$\varphi_{(3)}(x) = \frac{\pi[\gamma_n^{(3)}]^{1/2}}{nL} \int_0^x f^{1/2}(x') \psi(x') dx', \quad (30)$$

where  $\psi$  is defined by

$$\psi = 1 - v/2\gamma_n^{(3)}, \quad (31)$$

and  $\gamma_n^{(3)}$  is the third-order WKB eigenvalue that satisfies

$$0 = \gamma_n^{(3)} - n[\gamma_n^{(3)}]^{1/2} - A^{(3)}. \quad (32)$$

Note that the phase function  $\varphi_{(3)}$  has been defined so that its range is  $[0, \pi]$  when its domain is restricted to  $[0, l]$ . We also introduce a new dependent variable  $w^{(3)}$  which is related to the original  $y$  by

$$w^{(3)} = \left( \frac{d\varphi_{(3)}}{dx} \right)^{1/2} y. \quad (33)$$

In terms of these new variables, the differential equation (1) has precisely the same form as Eq. (9):

$$\frac{d^2 w^{(3)}}{d\varphi_{(3)}^2} + \frac{n^2 \lambda_n}{\gamma_n^{(3)}} w^{(3)} = v^{(3)} w^{(3)}, \quad (34)$$

where the "potential"  $v^{(3)}$  is given by

$$v^{(3)} = \alpha^{(3)} - \beta^{(3)} (n^2 \lambda_n / \gamma_n^{(3)}), \quad (35)$$

and

$$\alpha^{(3)} = \frac{n^2}{4\psi^2 \gamma_n^{(3)}} \left[ 4v - \frac{\ddot{v}}{\psi \gamma_n^{(3)}} - \frac{3}{4} \left( \frac{\dot{v}}{\psi \gamma_n^{(3)}} \right)^2 \right], \quad (36)$$

$$\beta^{(3)} = (v/\psi^2 \gamma_n^{(3)}) (1 - v/4\gamma_n^{(3)}). \quad (37)$$

The "dots" that appear in Eq. (36) refer (as in the rest of the paper) to differentiation with respect to  $\varphi$ . Note that  $\alpha^{(3)}$  and  $\beta^{(3)}$  depend only on the potential  $f$ , not on the (as yet) unknown eigenvalue  $\lambda_n$ .

Since Eq. (34) has precisely the same form as Eq. (9) (only the names of the variables have changed) all of the analysis of Sec. II can be applied directly to this case as well. In particular, since the potential  $v^{(3)}$  is small (of order  $\epsilon^4$  when  $\lambda_n$  is sufficiently close to the exact eigenvalue) the functions  $w_n^{(3)} = (2/\pi)^{1/2} \sin(n\varphi_{(3)})$  are good approximate solutions to Eq. (34). They are the third-order WKB functions that are orthonormal with respect to integrals over  $\varphi_{(3)}$  and have eigenvalues  $\lambda_n = \gamma_n^{(3)}$ . Using the  $w_n^{(3)}$  as trial functions in the variational principle, Eq. (6), we obtain the following third-order variational expression for the eigenvalues

$$\mu_n^{(3)} = \gamma_n^{(3)} (1 + v_{nn}^{(3)}/n^2), \quad (38)$$

where  $v_{nn}^{(3)}$  is the integral of  $v^{(3)} [w_n^{(3)}]^2$  with respect to  $\varphi_{(3)}$ . Unlike the first-order case,  $v_{nn}^{(3)}$  depends linearly on the eigenvalue. Thus introducing  $\alpha_{nn}^{(3)}$  and  $\beta_{nn}^{(3)}$  as the  $\varphi_{(3)}$  integrals of  $\alpha^{(3)} [w_n^{(3)}]^2$  and  $\beta^{(3)} [w_n^{(3)}]^2$ , respectively, we obtain the following expression for the third-order variational eigenvalue:

$$\mu_n^{(3)} = \gamma_n^{(3)} (n^2 + \alpha_{nn}^{(3)}) / n^2 (1 + \beta_{nn}^{(3)}). \quad (39)$$

Each of the terms on the right side of Eq. (39) is determined by straightforward calculation from the original potential  $f$ . It is appropriate to point out that each step of the analysis carried out here for the case of third-order WKB functions, could just as well have been accomplished for  $N$ th-order WKB functions. There will exist a reformulation of Eq. (1) which is exactly analogous to Eq. (34) for each order of WKB approximation. From there it follows that an improved approximation for the eigenvalue will be given for each WKB order by an expression having exactly the same form as Eq. (39).

How accurate is the approximate eigenvalue  $\mu_n^{(3)}$ ? A primary motivation for deriving the eigenvalue approximation, Eq. (39), via Eq. (34) is that this form of the equation allows us easy access to the perturbation theory techniques from which the error term may be evaluated. As we have shown in Sec. II, Eq. (20) gives the difference between the exact and approximate eigenvalue for this equation. Thus the exact eigenvalue  $\lambda_n$  is related to the third-order variational approximation  $\mu_n^{(3)}$  by

$$\lambda_n = \mu_n^{(3)} + E_n^{(3)}, \quad (40)$$

where  $E_n^{(3)}$  is given [in analogy with Eq. (20)] to lowest order in  $\epsilon$  by

$$E_n^{(3)} = \frac{\sigma_n \gamma_n^{(3)} (dv^{(3)}(0))^2}{n^4 (d\varphi_{(3)})^2}. \quad (41)$$

This expression can also be rewritten in the following form in terms of the more familiar variables

$$E_n^{(3)} = \frac{\sigma_n}{16n^6} \left( 2v(0)\dot{v}(0) - \frac{d^3 v(0)}{d\varphi^3} \right)^2 + O(\epsilon^{11}). \quad (42)$$

Thus the third-order variational estimate of the eigenvalue  $\mu_n^{(3)}$  differs from the exact eigenvalue by terms of order  $\epsilon^{10}$ ; and, this error term varies with the mode number as  $n^{-6}$ . The error in the third-order variational estimate is expected, therefore, to have the same  $n$ -dependence as the error of the seventh-order WKB eigenvalues and to be smaller by a factor of order  $\epsilon^2$ . The ninth-order WKB eigenvalues are expected to be more accurate than the third-order variational estimates for sufficiently large values of  $n$ , but are expected to be less accurate for small  $n$  values with most potentials. We point out that the variational estimate based on the  $N$ th-order WKB eigenfunctions will have an error term that has exactly the same form as Eq. (41). Since the  $N$ th-order potential  $v^{(N)}$  should be of order  $\epsilon^{N+1}$ , the error term for the  $N$ th-order variational estimate  $E_n^{(N)}$  is expected to be of order  $\epsilon^{2N+4}$ .

The expression, Eq. (39), for  $\mu_n^{(3)}$  has an interesting formal application. The difference between  $\mu_n^{(3)}$  and the exact eigenvalue has been shown to be of order  $\epsilon^{10}$ . Thus we may obtain from Eq. (39) an expression for the exact eigenvalue  $\lambda_n$  which is correct through order  $\epsilon^6$ . Expanding  $\mu_n^{(3)}$  to this order we find

$$\lambda_n = n^2 + v_{nn} + \frac{\dot{v}^2(0)}{n^2} \left( \frac{\pi^2}{48} - \frac{5}{16n^2} \right) + O(\epsilon^7). \quad (43)$$

If we compare this expression for  $\lambda_n$  with that given in Eqs. (16) and (20) we find that the infinite sum  $\sigma_n$  of Eq. (20) is

TABLE I. An example of the eigenvalue estimates for the case  $f(x) = (x + \pi)^4$ .

$n$	$\gamma_n^{(3)}$	$\gamma_n^{(5)}$	$\mu_n$	$\mu_n^{(3)}$	$\lambda_n$
1	0.856539	1.19301	0.925869	0.928280	0.924915
2	3.86086	3.96416	3.89760	3.89758	3.89727
3	8.86155	8.90731	8.88448	8.88448	8.88444
4	15.8618	15.8874	15.8774	15.8774	15.8774
5	24.8619	24.8782	24.8731	24.8732	24.8732
10	99.8620	99.8661	99.8656	99.8656	99.8654
20	399.862	399.863	399.863	399.863	399.863
40	1599.86	1599.86	1599.86	1599.86	1599.86

replaced by  $\pi^2/48 - 5/16n^2$ . Since these expressions must be the same to this order, it follows that the sum must be given by this simple expression [as indicated in the second equality in Eq. (21)]. We do not know how to evaluate this sum in any other way. We have verified that this expression for the sum is correct numerically for a wide range of  $n$ , and that the limit  $n \rightarrow \infty$  is also correct analytically.

## V. AN EXAMPLE

A numerical example will illustrate the accuracy of the various eigenvalue estimates discussed here. Consider the differential equation (1) on the domain  $[0, \pi]$  with  $f(x) = (x + \pi)^4$ . The exact eigenvalues  $\lambda_n$  for this problem have been computed numerically (for small values of  $n$ ) by Bender and Orszag.<sup>2</sup> We compare in Table I these exact eigenvalues with the various approximate eigenvalues considered in this paper: the third- and fifth-order WKB eigenvalues ( $\gamma_n^{(3)}$  and  $\gamma_n^{(5)}$ ) and the first- and third-order variational eigenvalues ( $\mu_n$  and  $\mu_n^{(3)}$ ). We have computed these various estimates by inserting this function  $f$  into the appropriate formulas for the estimates given in this paper. When necessary, the final integrations were performed numerically. These computations are straightforward and the details will not be given here. The variational estimates agree to within the numerical accuracy of the exact eigenvalues for  $n > 2$ . In contrast, the WKB estimates agree with the exact values to this accuracy only for  $n > 10$ . For the smallest values of  $n$  the accuracy of the lower-order estimates ( $\gamma_n^{(3)}$  and  $\mu_n$ ) is better than the accuracy of the higher-order estimates ( $\gamma_n^{(5)}$  and  $\mu_n^{(3)}$ ). This is presumably due to the fact that this

function  $f$  is not particularly slowly varying in the sense of Eqs. (11)–(12). The function  $v(x) = -2(7\pi^2/3)^2(x + \pi)^{-6}$  is fairly sharply peaked at  $x = 0$  and satisfies Eq. (11) only when  $\epsilon \approx 1$ , and Eq. (12) for  $k = 1$  when  $\epsilon \approx 1.7$  and for  $k = 2$  when  $\epsilon \approx 2.4$ . This example shows that the variational estimates are considerably more accurate than the WKB estimates for small values of  $n$ . This example is also an indication that the variational estimates are probably more “robust” in dealing with potentials that are only moderately slowly varying.

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<sup>1</sup>See, for example, P. M. Morse, and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Sec. 9.4.

<sup>2</sup>See, for example, C. M. Bender, and S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1978), pp. 490–493.

<sup>3</sup>The conditions in Eqs. (11)–(13) are somewhat stronger than needed. It is probably sufficient to bound the average values of  $v$ ,  $v'$ , and  $v''$ ; however, the analysis is more straightforward using these point-wise bounds.

<sup>4</sup>See, for example, Ref. 1, Sec. 9.1.

<sup>5</sup>See, for example, N. Fröman and P. O. Fröman, *Ann. Phys. (NY)* **163**, 215 (1985) and references therein.