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Author

Adams, John E.

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Semiclassical Eigenvalues for
Potential Functions Defined on a
Finite Interval^{*}

John E. Adams and William H. Miller[†]

Department of Chemistry, and Materials and Molecular
Research Division of the Lawrence Berkeley Laboratory,
University of California, Berkeley, CA 94720

Abstract

It is shown that the usual WKB quantum condition for one-dimensional potentials should be modified for problems defined on the finite interval (a,b) by adding the "correction" $\Delta V(x) = \frac{\hbar^2}{8m} \left(\frac{\pi}{b-a}\right)^2 / \cos^2\left[\frac{\pi}{b-a} \left(x - \frac{a+b}{2}\right)\right]$ to the actual potential. Numerical application shows the modified quantum condition to be a considerable improvement over the usual (i.e., un-modified) equation.

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I. Introduction

The ordinary WKB approximation¹ for the one-dimensional Schrödinger equation,

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) - E\right)\psi(x) = 0 \quad , \quad (1.1)$$

is appropriate if the domain of x is the entire real axis, $-\infty < x < +\infty$.

If $V(x)$ is a potential well, as in Figure 1a, then WKB, or semiclassical eigenvalues are determined by the Bohr-Sommerfeld quantum condition

$$\left(n + \frac{1}{2}\right)\pi = \int_{x_<}^{x_>} dx \sqrt{2m[E - V(x)]/\hbar^2} \quad , \quad (1.2)$$

for $n = 0, 1, 2, \dots$. If $V(x)$ is of the type corresponding to a scattering situation, as in Figure 1b, then it is the phase shift η which is of interest, and the WKB approximation for it is

$$\eta = \frac{\pi}{4} + \lim_{x \rightarrow \infty} \left[-kx + \int_{x_<}^x dx' \sqrt{2m[E - V(x')]/\hbar^2} \right] \quad . \quad (1.3)$$

Eqs. (1.2) and (1.3) are not strictly applicable, however, if the domain of x is not the whole line $(-\infty, +\infty)$. This situation most commonly arises when treating the radial Schrödinger equation of a spherically symmetric two-body problem. Here the coordinate (now called r) is restricted to the semi-infinite interval $(0, \infty)$, and as Langer² has shown, Eqs. (1.2) and (1.3) are modified by having the "correction term" $\frac{\hbar^2}{8mr^2}$ added to the potential V .

In this paper we show how Eq. (1.2) is modified when the domain of x is restricted to a finite interval (a,b) . (The notion of phase shift, and therefore Eq. (1.3), does not arise when dealing with a finite interval.) Section II first reviews Langer's idea of mapping a given domain onto the whole line $(-\infty, +\infty)$ and also the fact, emphasized by Fröman and Fröman,³ that this does not lead to a unique modification of Eqs. (1.2) and (1.3).

In Section III we show how a unique modification of Eq. (1.2) can be defined for the case of a finite interval, and Section IV describes the results obtained with this modified quantum condition for a harmonic oscillator confined to a finite interval. This example has specific relevance to treating frequency doubling in wave guides⁴ and has been the subject of recent quantum mechanical calculations.⁵ Comparison of the results of our modified WKB eigenvalue equation with the exact quantum mechanical values show it to be quite accurate and a considerable improvement over the unmodified quantum condition, Eq. (1.2).

II. Langer-Type Transformations; Non-Uniqueness

Suppose the Schrödinger equation (1.1) is defined on the finite interval $a \leq x \leq b$. Eq. (1.2) is then not strictly applicable, according to Langer,² and his solution to the problem is to map the interval (a,b) onto the whole line $(-\infty, +\infty)$. Let the one-to-one function $z(x)$ be the mapping function; i.e.,

$$z(a) = -\infty$$

$$z(b) = +\infty ,$$

and

$$z'(x) > 0$$

for all $x \in (a,b)$. It is then a straight-forward (but tedious) matter to convert the Schrödinger equation in x , Eq. (1.1), into an equivalent one in z and then to apply the WKB eigenvalue condition, Eq. (1.2), to the transformed equation. As Fröman and Fröman³ show in general, this leads to a quantum condition identical to Eq. (1.2) with the following "correction" $\Delta V(x)$ added to $V(x)$:

$$\Delta V(x) = -\frac{\hbar^2}{2m} z'(x)^{1/2} \frac{d^2}{dx^2} z'(x)^{-1/2} ; \quad (2.1)$$

i.e., the modified quantum condition is

$$(n + \frac{1}{2})\pi = \int_{x_<}^{x_>} dx \sqrt{2m[E - V(x) - \Delta V(x)]/\hbar^2} . \quad (2.2)$$

In Langer's specific case, for example, $(a,b) \equiv (0,\infty)$, the mapping

function he uses is

$$z(x) = \ln x \quad . \quad (2.3)$$

It is then easy to show that Eq. (2.1) gives

$$\Delta V(x) = \frac{\hbar^2}{8mx^2} \quad , \quad (2.4)$$

the well-known Langer² correction term.

A disturbing feature of this approach, however, is that the correction $\Delta V(x)$ is not invariant to the choice of mapping function.³ For the semi-infinite interval $(0, \infty)$, for example, another choice of mapping function is

$$z(x) = x - \frac{1}{x} \quad ; \quad (2.5)$$

clearly $x \in (0, \infty)$ maps onto $z \in (-\infty, +\infty)$ and $z'(x) > 0$. For this mapping function, however, Eq. (2.1) gives

$$\Delta V(x) = \frac{\hbar^2}{2m} \frac{3}{(1+x^2)^2} \quad , \quad (2.6)$$

which is considerably different from Langer's correction term.

For the finite interval (a, b) there are also a variety of choices of mapping functions. One which is similar in spirit to Langer's, Eq. (2.3), is

$$z(x) = \ln \left(\frac{x-a}{b-x} \right) \quad , \quad (2.7)$$

and from Eq. (2.1) one finds

$$\Delta V(x) = \frac{\hbar^2}{8m} \frac{(b-a)^2}{(x-a)^2(b-x)^2} \quad (2.8)$$

for this mapping function. $\Delta V(x)$ in Eq. (2.8) is similar to the Langer correction, Eq. (2.4), in that near the ends of the interval it takes the Langer form:

$$\lim_{x \rightarrow a} \frac{\hbar^2}{8m} \frac{(b-a)^2}{(x-a)^2(b-x)^2} = \frac{\hbar^2}{8m(x-a)^2} \quad (2.9a)$$

$$\lim_{x \rightarrow b} \frac{\hbar^2}{8m} \frac{(b-a)^2}{(x-a)^2(b-x)^2} = \frac{\hbar^2}{8m(b-x)^2} \quad (2.9b)$$

There are other choices for the mapping function, however, and they give different results for $\Delta V(x)$.

How then does one choose one mapping function over another? For the semi-infinite interval, why is Langer's correction, Eq. (2.4), to be preferred over any other (e.g., that of Eq. (2.6))? Our answer to the dilemma is that one chooses the mapping function, and therefore the correction term $\Delta V(x)$, so that the correct quantum mechanical result is obtained if the potential V is set to zero.

For the semi-infinite interval, for example, this criterion selects the Langer correction term uniquely: for $V(x) \equiv 0$, the phase shift should be zero, so that one should have

$$\eta = \frac{\pi}{4} + \lim_{x \rightarrow \infty} \left[-kx + \int_{x_0}^x dx' \sqrt{2m[E - \Delta V(x')]/\hbar^2} \right] \equiv 0, \quad (2.10)$$

and only Langer's correction, $\Delta V(x)$ of Eq. (2.4), satisfies this.⁶ Other corrections do not in general give $\eta \equiv 0$ when $V \equiv 0$, which is clearly unphysical, and our point of view is that this is the primary reason why Langer's correction is the preferred one.

III. The Correction Term for Finite Intervals

The strategy described at the end of the preceeding section is what is now followed to find the "best" $\Delta V(x)$ for the finite interval (a,b) . Thus $V(x)$ is set to zero in the modified WKB quantum condition, Eq. (2.2), so that it reads

$$(n + \frac{1}{2})\pi = \int_{x_<}^{x_>} dx \sqrt{2m[E - \Delta V(x)]/\hbar^2} \quad , \quad (3.1)$$

and we seek the function $\Delta V(x)$ for which Eq. (3.1) gives the correct quantum mechanical eigenvalues for this case that $V(x) \equiv 0$ for $x \in (a,b)$; these, of course, are the "particle-in-a-box" eigenvalues,

$$E_n = \frac{\hbar^2}{2m} \left[\frac{(n+1)\pi}{b-a} \right]^2 \quad , \quad (3.2)$$

$n = 0, 1, 2, \dots$

This problem can be solved by using the RKR inversion method,⁷ a procedure which allows one to construct the potential function which gives rise, within the WKB approximation, to a specific set of eigenvalues. Assuming that $\Delta V(x)$ is symmetric about the mid-point of the interval, $\frac{a+b}{2}$, the RKR formula is⁷

$$x - \frac{a+b}{2} = \sqrt{\frac{\hbar^2}{2m}} \int_{-1/2}^{\infty} dn [\Delta V - E(n)]^{-1/2} \quad , \quad (3.3)$$

where the upper limit of the integral is the zero of the radicand, and where $E(n)$ is given by Eq. (3.2). Carrying out this integral gives x in terms of ΔV ,

$$x - \frac{a+b}{2} = \frac{b-a}{\pi} \cos^{-1} \left[\frac{\pi}{b-a} \sqrt{\frac{\hbar^2}{8m\Delta V}} \right] ,$$

which can be inverted to give $\Delta V(x)$:

$$\Delta V(x) = \frac{\hbar^2}{8m} \frac{\left(\frac{\pi}{b-a}\right)^2}{\cos^2 \left[\frac{\pi}{b-a} \left(x - \frac{a+b}{2}\right) \right]} \quad (3.4)$$

Eq. (3.4) is the desired correction term for the finite interval (a,b). To summarize, for any potential $V(x)$ defined on the (a,b) interval, the modified WKB eigenvalue condition is

$$\left(n + \frac{1}{2}\right)\pi = \int_{x_<}^{x_>} dx \sqrt{2m[E - V(x) - \Delta V(x)]/\hbar^2} , \quad (3.5)$$

with $\Delta V(x)$ given by Eq. (3.4). By construction, if $V(x) \equiv 0$ then Eq. (3.5) gives the correct quantum eigenvalues, Eq. (3.2). Without the correction $\Delta V(x)$ the WKB eigenvalues for $V = 0$ would be

$$E_n = \frac{\hbar^2}{2m} \left[\frac{\left(n + \frac{1}{2}\right)\pi}{b-a} \right]^2 , \quad (3.6)$$

$n = 0, 1, 2, \dots$, which are quite poor for small n ; for $n = 0$, it is off by a factor of 4, and for $n = 1$ by a factor of 1.8.

It is interesting to note that our correction in Eq. (3.4) assumes the Langer form in the limit that x is close to one of the end points; e.g.,

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$$\Delta V(x) = \frac{\hbar^2}{8m} \frac{\left(\frac{\pi}{b-a}\right)^2}{\cos^2\left[\frac{\pi}{b-a}\left(x-a - \frac{b-a}{2}\right)\right]}$$

$$= \frac{\hbar^2}{8m} \frac{\left(\frac{\pi}{b-a}\right)^2}{\cos^2\left[\frac{\pi}{b-a}(x-a) - \frac{\pi}{2}\right]}$$

$$= \frac{\hbar^2}{8m} \frac{\left(\frac{\pi}{b-a}\right)^2}{\sin^2\left[\frac{\pi(x-a)}{b-a}\right]}$$

$$\longrightarrow \frac{\hbar^2}{8m(x-a)^2}, \quad (3.7)$$

as $x \rightarrow a$; it has a similar limit as $x \rightarrow b$. Finally, one notes that in the special case that $(a,b) \equiv (0,\infty)$, Eq. (3.4) becomes

$$\Delta V(x) = \lim_{b \rightarrow \infty} \frac{\hbar^2}{8m} \frac{\left(\frac{\pi}{b}\right)^2}{\cos^2\left(\frac{\pi x}{b} - \frac{\pi}{2}\right)}$$

$$= \lim_{b \rightarrow \infty} \frac{\hbar^2}{8m} \frac{\left(\frac{\pi}{b}\right)^2}{\sin^2\left(\frac{\pi x}{b}\right)}$$

$$= \frac{\hbar^2}{8mx^2};$$

i.e., it becomes the Langer correction if (a,b) is the semi-infinite limit.

IV. Example: Harmonic Oscillator in a Box

As an example of the modified WKB eigenvalue condition, Eqs. (3.4) and (3.5), we consider a harmonic oscillator of unit mass ($m = 1$) defined on the interval $(-\frac{L}{2}, \frac{L}{2})$; i.e., the potential is $+\infty$ for $|x| > \frac{L}{2}$. The potential plus the correction term is

$$V(x) + \Delta V(x) = \frac{1}{2} \omega^2 x^2 + \frac{1}{8} \frac{(\pi/L)^2}{\cos^2(\frac{\pi x}{L})}, \quad (4.1)$$

where units are used such that $\hbar = 1$. For $L \rightarrow \infty$ the correction vanishes and the eigenvalues will be those of the ordinary harmonic oscillator,

$$\lim_{L \rightarrow \infty} E_n = (n + \frac{1}{2})\omega, \quad (4.2)$$

$$n = 0, 1, 2, \dots$$

while for $L \rightarrow 0$ one has $\Delta V(x) \gg V(x)$, so that the eigenvalues will be those determined by $\Delta V(x)$ alone,

$$\lim_{L \rightarrow 0} E_n = \frac{1}{2} \left[\frac{(n+1)\pi}{L} \right]^2. \quad (4.3)$$

$$n = 0, 1, 2, \dots$$

A quantum mechanical calculation of these eigenvalues as a function of L has recently been reported,⁵ and this provides an excellent test of the modified WKB quantum condition. Setting $\omega = \frac{1}{2}$, Table I and Figure 2 show the ground ($n = 0$) and first excited state ($n = 1$) eigenvalues as a function of L , the box size.

One sees that the modified WKB eigenvalues are in quite good agreement

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with the exact quantum mechanical ones and certainly a major improvement over the ordinary WKB values for small L . There is an intermediate range of L for which the ordinary WKB eigenvalues are slightly more accurate than the modified ones, though both converge rapidly to the correct results as $L \rightarrow \infty$.

V. Concluding Remarks

The main result of the paper is the correction term, $\Delta V(x)$ of Eq. (3.4), which should be added to the actual potential when applying the WKB quantum condition to a problem confined to the finite interval (a,b) . For the special case $(a,b) = (0,\infty)$ it becomes the usual Langer correction, Eq. (2.4).

The example discussed in Section IV shows that that modified WKB quantum condition is a substantial improvement over the un-modified WKB equation and for this example gives good agreement with the quantum mechanical eigenvalues.

References

- * Supported by the National Science Foundation under Grant CHE76-22621.
- † Camille and Henry Dreyfus Teacher-Scholar.
- 1. See, for example, P. M. Morse and H. Feshbach, Methods of Theoretical Physics, McGraw-Hill, N.Y., Vol. II, 1953, pp. 1092-1106.
- 2. R. E. Langer, Phys. Rev. 51, 669 (1937).
- 3. N. Fröman and P. O. Fröman, Nuovo Cimento 20, 121 (1974).
- 4. R. I. Masel, private communication.
- 5. A. Consortini and B. R. Frieden, Nuovo Cimento 35, 153 (1976).
- 6. Eq. (2.10) applies only to the case of angular momentum $\ell = 0$ for a radial problem. To conclude that the Langer correction is unique, it is actually necessary to require for all ℓ that $\eta_\ell \equiv 0$ if $V(r) \equiv 0$.
- 7. See, for example, E. A. Mason and L. Monchick, Adv. Chem. Phys. 12, 351 (1967).

Table I. Eigenvalues for a Harmonic Oscillator in a Box.^(a)

<u>Quantum Number</u>	<u>$L/\sqrt{2}$</u>	<u>WKB^(b)</u>	<u>Quantum^(c)</u>	<u>Modified WKB^(d)</u>
0	0.5	2.47	9.87	9.88
0	1	0.64	2.48	2.48
0	2	0.25	0.65	0.67
0	3	0.25	0.34	0.38
0	4	0.25	0.27	0.30
1	0.5	22.21	39.48	39.55
1	1	5.57	9.89	9.90
1	2	1.47	2.54	2.54
1	3	0.82	1.25	1.26
1	4	0.75	0.88	0.90

(a) Potential parameters as defined in Section IV.

(b) Results of the ordinary (i.e., un-modified) WKB quantum condition, Eq. (1.2).

(c) Results of reference 5.

(d) Results of the modified WKB quantum condition, Eqs. (3.4) and (3.5).

Figure Captions

Figure 1. (a) A typical potential function for which bound state eigenvalues exist. (b) A typical one-dimensional scattering potential. In both cases $x_<$ and $x_>$ denote classical turning points, the roots of the equation $V(x) = E$.

Figure 2. Eigenvalues of the ground ($n = 0$) and first excited state ($n = 1$) for a harmonic oscillator of frequency $\omega = \frac{1}{2}$ in a box of length L . The points represent the exact quantum mechanical values of reference 5, the solid curves the values calculated via the modified WKB quantum condition, Eqs. (3.4)-(3.5), and the dashed lines the results given by the ordinary unmodified WKB quantum condition, Eq. (1.2).

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Fig. 1

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Fig. 2

0 0 1 3 0 0 1 3 7

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