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Higher-order calculation of transmission below the potential barrier

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In extending the Miller-Good modified WKB approximation to include the higher-order terms, a divergence was introduced. Because of this divergence, the approximation was limited to energies above the potential barrier. With this divergence removed, the modified WKB method is no longer limited to energies above the potential barrier. In order to demonstrate this method, we calculate the transmission coefficients for energies below the peak of the potential barrier and show that the higher-order terms are essential to the approximation.

I. INTRODUCTION

The conventional WKB approximation is widely known for its usefulness in solving simple barrier-penetration problems. However, as Ford *et al.*[1] pointed out, the conventional WKB method tends to break down as the energy approaches the potential-barrier top.

Miller and Good[2] proposed a modified WKB method in which the solutions of a model Schrödinger equation that can be solved exactly and resembles the actual Schrödinger equation would be used as the basis of the approximation. The reader is referred to their paper for details. However, the modified WKB method was only utilized to zeroth order in $\hbar^2$ because of divergences in the higher-order terms. Using the method developed by Lu and Measure[3] to remove the divergences in the higher-order terms, a divergence at the maximum point of the potential barrier was introduced. This divergence limits the approximation to energies above the barrier top where there are no real classical turning points, and hence there is no maximum point on the path of integration. Using the modified WKB method to first order in $\hbar^2$, we calculated the transmission coefficients above the potential barrier[4] and obtained agreement with the numerical results to at least four significant figures. This indicated how essential the higher-order terms are to the approximation.

For the case of penetration below the potential barrier, there are two classical turning points and one maximum point lying between the turning points. In order to remove the divergence at the maximum point, we start with the basic contour integral representation and then derive a formula which can be applied to the case of "penetration through the barrier." In Sec. II, this formula is derived in general terms. Using the Eckart potential as an example in Sec. III, we calculate the transmission coefficients for energies below the barrier, and the results are shown to be in agreement with the numerical results as presented in Table I. Thus the barrier-penetration problem can be solved using the modified WKB method with excellent results even for energies near the top of the potential barrier.

II. METHOD OF APPROXIMATION

In general, we wish to solve the Schrödinger equation

$$\left[\frac{d^2}{dx^2}+\frac{P_1^{\,2}(x)}{\hbar^2}\right]\psi(x)=0 \tag{1}$$

TABLE I. Transmission coefficients T for various energies W: (a) modified WKB approximation to zeroth order in $\hbar^2$, (b) modified WKB approximation to first order in $\hbar^2$, (c) exact results. As mentioned in the text, the transmission coefficients are for $W < W_C$, where $W_C = 3.8$ is the maximum of the potential barrier.

		T	
W	(a)	(b)	(c)
2.000	0.41731×10^{-6}	0.49264×10^{-6}	0.48942×10^{-6}
2.125	0.28143×10^{-5}	0.33222×10^{-5}	0.33227×10^{-5}
2.250	0.12130×10^{-4}	0.14320×10^{-4}	0.14326×10^{-4}
2.375	0.42627×10^{-4}	0.50321×10^{-4}	0.50344×10^{-4}
2.500	0.13204×10^{-3}	0.15586×10^{-3}	0.000155
2.625	0.37411×10^{-3}	0.44161×10^{-3}	0.000418
2.750	0.99029×10^{-3}	0.11688×10^{-2}	0.001169
2.875	0.24813×10^{-2}	0.29279×10^{-2}	0.002929
3.000	0.005934	0.006998	0.007001
3.125	0.013607	0.016024	0.016031
3.250	0.029928	0.035141	0.035157
3.375	0.062836	0.073347	0.073379
3.500	0.124384	0.143612	0.143670
3.625	0.227300	0.257753	0.257842

for a given potential $V(x)$, where

$$P_1^2(x)=t_1(x)=2m[W-V(x)]\,. \tag{2}$$

The classical turning points correspond to the condition $P_1(x_i)=0$, where x_i is the ith turning point.

We now construct a model potential $U(s)$ which is qualitatively similar to $V(x)$ and whose Schrödinger equation can be solved exactly. Thus we have

$$\left[\frac{d^2}{ds^2}+\frac{P_2^2(s)}{\hbar^2}\right]\phi(s)=0\,, \tag{3}$$

where

$$P_2^2(s)=t_2(s)=E-U(s) \tag{4}$$

and E is a parameter to be determined. The turning points of the model potential correspond to the condition $P_2(s_i)=0$, where s_i is the ith turning point of the model problem. Both the actual and the model potential must have the same number of turning points.

The solution to the Schrödinger equation of the actual potential is given by

$$\psi(x)=[s'(x)]^{-1/2}\,\phi(s(x))\,. \tag{5}$$

Substituting Eqs. (3) and (5) into Eq. (1), we obtain to zeroth order in $\hbar^2$ (see Ref. 2)

$$\int_{s_1}^{s_2}P_2(s)ds=\int_{x_1}^{x_2}P_1(x)dx \tag{6}$$

and to first order in $\hbar^2$ (see Ref. 3)

$$\int_{s_1}^{s_2}P_2ds-\frac{\hbar^2}{16}\oint\left(\frac{2P_2''}{P_2^2}-\frac{3P_2'^2}{P_2^3}\right)ds =\int_{x_1}^{x_2}P_1dx-\frac{\hbar^2}{16}\oint\left(\frac{2P_1''}{P_1^2}-\frac{3P_1'^2}{P_1^3}\right)dx\,, \tag{7}$$

where x_1, x_2 and s_1, s_2 are the respective turning points. The contour of the integrals is taken in a clockwise direction around the turning points as shown in Fig. 1. Using

$$\oint u\,dv=-\oint v\,du \tag{8}$$

Eq. (7) can be reduced to

$$\int_{s_1}^{s_2}P_2ds+\frac{\hbar^2}{12}\oint\left(\frac{t_2''}{t_2'^2t_2^{1/2}}-\frac{t_2'''}{t_2't_2^{1/2}}\right)ds =\int_{x_1}^{x_2}P_1dx+\frac{\hbar^2}{12}\oint\left(\frac{t_1''}{t_1'^2t_1^{1/2}}-\frac{t_1'''}{t_1't_1^{1/2}}\right)ds\,. \tag{9}$$

While the divergences at the turning points have been removed, another divergence at $t'=0$ has been introduced. Converting the contour integrals to definite integrals, we obtain

$$\int_{s_1}^{s_2}P_2ds+\frac{\hbar^2}{24}\int_{s_1}^{s_2}\left(\frac{t_2''^2}{t_2'^2t_2^{1/2}}-\frac{t_2'''}{t_2't_2^{1/2}}\right)ds =\int_{x_1}^{x_2}P_1dx+\frac{\hbar^2}{24}\int_{x_1}^{x_2}\left(\frac{t_1''^2}{t_1'^2t_1^{1/2}}-\frac{t_1'''}{t_1't_1^{1/2}}\right)dx \tag{10}$$

with the understanding that $t_1'\neq0$ and $t_2'\neq0$ through-

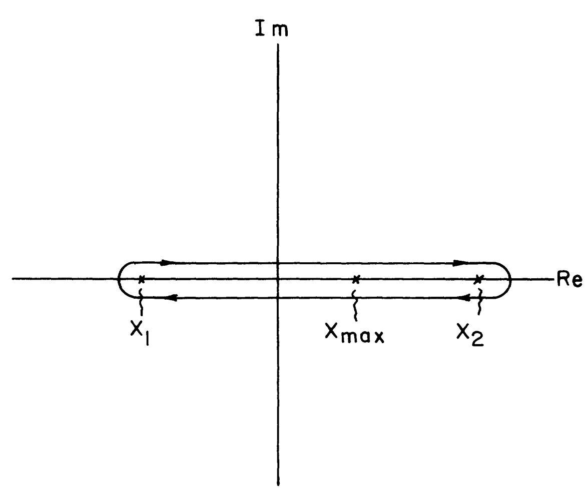

FIG. 1. The contour of integration.

out their ranges of integration (see Ref. 3 for details). For energies above the potential barrier, there can be no real turning points, and hence $t_1'\neq 0$ and $t_2'\neq 0$ throughout their respective ranges of integration, so that Eq. (10) can be used. Integrating Eq. (9) by parts one more time using Eq. (8) yields

$$\int_{s_1}^{s_2} P_2 ds + \frac{\hbar^2}{24} \oint t_2^{1/2}\left(\frac{t_2^{(\mathrm{iv})}}{t_2'^2} - \frac{4t_2'''t_2''}{t_2'^3} + \frac{3t_2''^3}{t_2'^4}\right) ds = \int_{x_1}^{x_2} P_1 dx + \frac{\hbar^2}{24} \oint t_1^{1/2}\left(\frac{t_1^{(\mathrm{iv})}}{t_1'^2} - \frac{4t_1'''t_1''}{t_1'^3} + \frac{3t_1''^3}{t_1'^4}\right) dx, \tag{11}$$

where the Roman numerals inside the bracket indicate the number of times the function has been differentiated. Now in a complex plane, one can always choose a contour of integration such that $x_{\max}$ or $s_{\max}$ is enclosed by the contour. However, the path of integration of the definite integral is always on the real axis which passes through $x_{\max}$ or $s_{\max}$. Therefore extreme care must be exercised in converting the contour integrals to definite integrals. We arbitrarily choose the points δ_1, δ_2 and γ_1, γ_2 such that

$$0<\delta_1<x_{\max}-x_1\,, \tag{12a}$$

$$0<\delta_2<x_2-x_{\max}\,, \tag{12b}$$

$$0<\gamma_1<s_{\max}-s_1\,, \tag{12c}$$

$$0<\gamma_2<s_2-s_{\max}\,. \tag{12d}$$

By converting the contour integrals in Eq. (11) to definite integrals and subdividing the intervals along the path of integration, we can isolate the divergent integral. The integrals can be integrated by parts so that Eq. (11) can be rewritten as

$$\int_{s_1}^{s_2} P_2 ds + \frac{\hbar^2}{12}\int_{s_1}^{s_{\max}-\gamma_1}\left(\frac{t_2^{(\mathrm{iv})}}{t_2'^2} - \frac{4t_2'''t_2''}{t_2'^3} + \frac{3t_2''^3}{t_2'^4}\right) t_2^{1/2} ds + \frac{\hbar^2}{12}\int_{s_{\max}+\gamma_2}^{s_2}\left(\frac{t_2^{(\mathrm{iv})}}{t_2'^2} - \frac{4t_2'''t_2''}{t_2'^3} + \frac{3t_2''^4}{t_2'^4}\right) t_2^{1/2} ds + \frac{\hbar^2}{12} J_2$$
$$= \int_{x_1}^{x_2} P_1 dx + \frac{\hbar^2}{12}\int_{x_1}^{x_{\max}-\delta_1}\left(\frac{t_1^{(\mathrm{iv})}}{t_1'^2} - \frac{4t_1'''t_1''}{t_1'^3} + \frac{3t_1''^3}{t_1'^4}\right) t_1^{1/2} dx + \frac{\hbar^2}{12}\int_{x_{\max}+\delta_2}^{x_2}\left(\frac{t_1^{(\mathrm{iv})}}{t_1'^2} - \frac{4t_1'''t_1''}{t_1'^3} + \frac{3t_1''^3}{t_1'^4}\right) t_1^{1/2} dx + \frac{\hbar^2}{12} J_1\,, \tag{13}$$

where

$$J_1 = \left[\left(\frac{t_1'''}{t_1'^2} - \frac{t_1''^2}{t_1'^3}\right) t_1^{1/2} - \frac{1}{2}\,\frac{t_1''}{t_1' t_1^{1/2}}\right]\Bigg|_{x_{\max}-\delta_1}^{x_{\max}+\delta_2} - \frac{1}{4}\int_{x_{\max}-\delta_1}^{x_{\max}+\delta_2} \frac{t_1''}{t_1^{3/2}}\, dx\,, \tag{14a}$$

$$J_2 = \left[\left(\frac{t_2'''}{t_2'^2} - \frac{t_2''^2}{t_2'^3}\right) t_2^{1/2} - \frac{1}{2}\,\frac{t_2''}{t_2' t_2^{1/2}}\right]\Bigg|_{s_{\max}-\gamma_1}^{s_{\max}+\gamma_2} - \frac{1}{4}\int_{s_{\max}-\gamma_1}^{s_{\max}+\gamma_2} \frac{t_2''}{t_2^{3/2}}\, ds\,. \tag{14b}$$

It is obvious that the method employed should be independent of the choice of δ_1, δ_2 and γ_1, γ_2. This is true if all orders in $\hbar^2$ are included, but even to first order in $\hbar^2$ the dependence on the choice of δ_1, δ_2 and γ_1, γ_2 is so small as to be considered negligible. This will be shown to be true in Sec. III using the Eckart potential as an example.

While Eq. (13) is not rigorously derived here, we will see in Sec. III, using the Eckart potential as an example, that we can obtain excellent agreement with the numerical results even for energies near the top of the barrier. The method of removing the divergence in the higher-order terms is confirmed by the results shown in Table I. Thus the penetration problem can be solved by the modified WKB approximation.

Using Eq. (13), the parameter E can be determined so that an approximation of the wave function to first order in $\hbar^2$ is given by Eq. (5). The transmission coefficient is then given by

$$T = \frac{J_{\text{trans}}}{J_{\text{inc}}}\,, \tag{15}$$

where

$$J = \frac{\hbar}{2mi}\left[\psi^* \frac{d}{dx}\psi - \left(\frac{d}{dx}\psi^*\right)\psi\right]$$

and

$$\psi_{\text{trans}} \underset{\substack{x\to+\infty \\ s\to+\infty}}{=} [s'(x)]^{-1/2}\phi(s(x))\,,$$

$$\psi_{\text{inc}} \underset{\substack{x\to-\infty \\ s\to-\infty}}{=} [s'(x)]^{-1/2}\phi(s(x))\,.$$

The normalization constants for the wave functions are omitted since Eq. (15) only involves the ratio of the wave functions.

III. APPLICATION TO THE ECKART POTENTIAL

The Eckart potential as demonstrated in Refs. 2 and 4 is given as

$$V(x)=1.922e^x(1+e^x)^{-1}+11.2e^x(1+e^x)^{-2}\,. \tag{16}$$

The turning points are obtained from the condition $P_1(x_i)=0$ so that

$$y_1=\exp(x_1)=\frac{A-B}{C} \tag{17a}$$

and

$$y_2=\exp(x_2)=\frac{A+B}{C}\,, \tag{17b}$$

where

$$A=13.122-2W\,,$$

$$B=(13.122-44.8W)^{1/2}\,,$$

$$C=2(W-1.922)\,,$$

and

$$P_1^2(x)=t_1(x)=2[W-V(x)]\,.$$

The model potential is given by $U(s)=-s^2$ such that $P_2^2(s)=t_2(s)=E+s^2$ and the Schrödinger equation for the model potential is

$$\left(\frac{d^2}{ds^2}+\frac{E+s^2}{\hbar^2}\right)\phi(s)\,. \tag{18}$$

The exact solution $\phi(s)=D_n(z)$ is given by Whittaker and Watson[5] for $n=\frac{1}{2}(\pm iE-1)$ and $z=\sqrt{2}\,se^{i\pi/4}$. The asymptotic representation for $D_n(z)$ can be found in the appendix of Ref. 2. The turning points of the model potential correspond to the condition $P_2(s_i)=0$ and are given by

$$\left.\begin{aligned} s_1&=i|E|^{1/2}\\ s_2&=-i|E|^{1/2}\end{aligned}\right\}\ \text{for } E>0 \tag{19}$$

and

$$\left.\begin{aligned} s_1&=-|E|^{1/2}\\ s_2&=+|E|^{1/2}\end{aligned}\right\}\ \text{for } E<0\,. \tag{20}$$

The case when $E>0$ corresponds to penetration over the barrier, and the details can be found in Ref. 4.

The first term on the left-hand side of Eq. (13) can be integrated to give

$$\int_{s_1}^{s_2}P_2(s)ds=\int_{-|E|^{1/2}}^{|E|^{1/2}}(E+\sigma^2)^{1/2}d\sigma=\tfrac{1}{2}i|E|\pi\,,$$

and the sum of the higher-order terms on the left-hand side of Eq. (13) is zero (see Appendix). Thus Eq. (13) becomes

$$\begin{aligned}\tfrac{1}{2}|E|\pi=&-\int_{x_1}^{x_2}[-P_1^2(x)]^{1/2}dx-\frac{\hbar^2}{12}\int_{x_1}^{x_{\max}-\delta_1}\left(\frac{t_1^{(iv)}}{t_1'^2}-\frac{4t_1'''t_1''}{t_1'^3}+\frac{3t_1''^3}{t_1'^4}\right)(-t_1)^{1/2}dx\\ &-\frac{\hbar^2}{12}\int_{x_{\max}+\delta_2}^{x_2}\left(\frac{t_1^{(iv)}}{t_1'^2}-\frac{4t_1'''t_1''}{t_1'^3}+\frac{3t_1''^3}{t_1'^4}\right)(-t_1)^{1/2}dx-\frac{\hbar^2}{12}J_1\,,\end{aligned} \tag{21}$$

where

$$J_1=\left[\left(\frac{t_1'''}{t_1'^2}-\frac{t_1''^2}{t_1'^3}\right)(-t_1)^{1/2}+\frac{1}{2}\,\frac{t_1'''}{t_1'(-t_1)^{1/2}}\right]\Bigg|_{x_{\max}-\delta_1}^{x_{\max}+\delta_2}+\frac{1}{4}\int_{x_{\max}-\delta_1}^{x_{\max}+\delta_2}\frac{t_1''}{(-t_1)^{3/2}}\,. \tag{22}$$

Equations (21) and (22) are obtained by multiplying both sides of Eq. (13) by $-i$ bringing i inside the square root of the integrand on the right-hand side. The points δ_1, δ_2 and γ_1,γ_2 were arbitrarily chosen to be as follows:

$$\delta_1=\tfrac{1}{2}(x_{\max}-x_1)\,,\qquad \delta_2=\tfrac{1}{2}(x_2-x_{\max})\,,$$

$$\gamma_1=\tfrac{1}{2}(s_{\max}-s_1)\,,\qquad \gamma_2=\tfrac{1}{2}(s_2-s_{\max})$$

or

$$\delta_1=\tfrac{1}{3}(x_{\max}-x_1)\,,\qquad \delta_2=\tfrac{1}{3}(x_2-x_{\max})\,,$$

$$\gamma_1=\tfrac{1}{3}(s_{\max}-s_1)\,,\qquad \gamma_2=\tfrac{1}{3}(s_2-s_{\max})\,.$$

The integrals on the right-hand side of Eq. (21) were evaluated numerically using both sets of arbitrarily chosen points in order to determine the parameter E.

The transmission coefficient, using Eq. (15), becomes

$$T=(1+e^{|E|\pi})^{-1} \tag{23}$$

for both the zeroth- and the first-order approximation. However, E in Eq. (23) satisfies Eq. (6) to zeroth order in $\hbar^2$ and Eq. (13) to first order in $\hbar^2$.

As previously stated, the method employed in removing the divergence to obtain Eq. (13) should be independent of the choice of δ_1, δ_2 and γ_1,γ_2. This is true if all the higher-order terms of the approximation are included. But even to first order in $\hbar^2$, the dependence on the choice of δ_1, δ_2 and γ_1,γ_2 is so small that it can be considered negligible. For $W=2.000$, $T=0.49264296\times10^{-6}$ using $\delta_1=\frac{1}{3}(x_{\max}-x_1)$ and $\delta_2=\frac{1}{3}(x_2-x_{\max})$, while at the same energy $T=0.49264288\times10^{-6}$ using $\delta_1=\frac{1}{2}(x_{\max}-x_1)$ and

$\delta_2=\frac{1}{2}(x_2-x_{\max})$. For $W=3.625$, $T=0.2577528943$ using $\delta_1=\frac{1}{3}(x_{\max}-x_1)$ and $\delta_2=\frac{1}{3}(x_2-x_{\max})$, while at the same energy $T=0.2577528509$ using $\delta_1=\frac{1}{2}(x_{\max}-x_1)$ and $\delta_2=\frac{1}{2}(x_2-x_{\max})$.

The transmission coefficients obtained by the zeroth- and the first-order approximation together with the exact numerical results[6] are presented in Table I. The excellent agreement between the first-order approximation and the numerical results tends to confirm the method and indicates how essential the higher orders are to the approximation.

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APPENDIX

Here, we verify that the sum of the higher-order terms in $\hbar^2$ is exactly zero for the model part where $P_2{}^2=t_2=s^2-|E|$.

Since $E=-|E|$ and $t_2'=2s$, $t_2''=2$, and $t_2'''=t_2''''=0$, we label

$$I_1\equiv\int_{s_1}^{s_M-\xi}3t_2{}^{1/2}\frac{t_2''^3}{t_2'^4}\,ds$$

$$=\tfrac{3}{2}\int_{s_1}^{s_M-\xi}(\sigma^2-|E|)^{1/2}\frac{d\sigma}{\sigma^4}$$

$$=i\,\frac{(|E|-\xi^2)^{3/2}}{2|E|\,\xi^3},$$

$$I_2\equiv\int_{s_M+\epsilon}^{s_2}3t_2{}^{1/2}\frac{t_2''^3}{t_2'^4}\,ds$$

$$=i\,\frac{(|E|-\epsilon^2)^{3/2}}{2|E|\,\epsilon^3},$$

and

$$I_3=\left[\left(\frac{t_2'''}{t_2'^2}-\frac{t_2''^2}{t_2'^3}\right)t_2{}^{1/2}-\frac{t_2''}{2t_2't_2{}^{1/2}}\right]\Bigg|_{s_M-\xi}^{s_M+\epsilon}-\frac{1}{4}\int_{s_M-\xi}^{s_M+\epsilon}\frac{t_2''}{t_2{}^{3/2}}\,ds$$

$$=i\left[\frac{-(E-\sigma^2)^{1/2}}{2\sigma^3}+\frac{1}{2\sigma(|E|-\sigma^2)^{1/2}}\right]\Bigg|_{-\xi}^{\epsilon}-\frac{i}{2}\int_{-\xi}^{\epsilon}\frac{d\sigma}{(|E|-\sigma^2)^{3/2}}$$

$$=i\left[\frac{-(|E|-\epsilon^2)^{1/2}}{2\epsilon^3}+\frac{1}{2(|E|-\epsilon^2)^{1/2}}\left(\frac{1}{\epsilon}-\frac{\epsilon}{|E|}\right)-\frac{(|E|-\xi^2)^{1/2}}{2\xi^3}+\frac{1}{2(|E|-\xi^2)^{1/2}}\left(\frac{1}{\xi}-\frac{\xi}{|E|}\right)\right].$$

Here

$$I_1+I_2+I_3=i\left[(|E|-\xi^2)^{1/2}\left(\frac{|E|-\xi^2}{2|E|\xi^3}-\frac{1}{2\xi^3}+\frac{1}{2\xi|E|}\right)+(|E|-\epsilon^2)^{1/2}\left(\frac{|E|-\epsilon^2}{2|E|\epsilon}-\frac{1}{2\epsilon^3}+\frac{1}{2\epsilon|E|}\right)\right]$$

$$=0,$$

with ϵ and ξ being arbitrary as γ_1 and γ_2 given in text. Except for a proportionality constant, we see that $I_1+I_2+I_3$ corresponds to the higher-order contribution in $\hbar^2$ to the model side of Eq. (13).

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