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Higher-Order Corrections of the Modified WKB Approximation to the Solution of the Repulsive Singular Potential

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We extend the modified WKB approximation due to Miller and Good to the $\hbar^4$ order for the scattering case by the repulsive inverse-fourth-power potential. Instead of describing the higher-order terms by the phase-integral formula in terms of line integrals with a specific contour in a complex plane, we present the formula here in terms of definite integrals.

I. INTRODUCTION

In a recent note, we showed[1] that the modified WKB method as given by Miller and Good[2] is valid in regions where the ordinary WKB method fails to yield dependable results. This is specifically done in the low-energy region of the one-turning-point problem where we have exact phase shifts to compare with. It is in the low-energy region that the ordinary WKB method is known to fail.[3] The exact phase shifts[4,5] are mainly from the solution of Mathieu's equation at the low-energy and small-coupling-constant limit. So we see that the ordinary WKB method cannot be used for comparison with our results since it is not valid in the low-energy, small-coupling-constant limit for a highly singular potential such as $1/r^4$. Of course, the modified WKB method yields a correct approximation of the phase shifts at all energies. Now we are going to see how and to what extent the approximation is correct when compared with the regions where the exact results are available. This modified WKB method will be reduced to the ordinary WKB method at the high-energy limit. Therefore, we see that we get an approximation method which is valid at all energies. Previously we showed that the inclusion of the $\hbar^2$ term contributed to the results which were summarized in a table in Ref. 1. At that time, we argued that the higher-order terms must contribute to the results. We now include the $\hbar^4$ terms to demonstrate this fact.

The Schrödinger equation that we want to solve is of the form

$$\frac{d^2\psi}{dr^2}+\frac{p_1^{\,2}(r)}{\hbar^2}\psi=0\ , \tag{1a}$$

where we let

$$t_1(r)\equiv p_1^{\,2}=2E-[l(l+1)\hbar^2/r^2]-2g^2/r^4\ , \tag{1b}$$

and from the assumption that only a one-turning-point problem is discussed here, we take $g^2>0$. It is important to point out here that we are using a different definition of g^2 (with respect to Ref. 5 by $g^2/2$ in their notation). The Schrödinger equation whose solutions are known is given by

$$\frac{d^2\phi}{dS^2}+\frac{p_2^{\,2}}{\hbar^2}\phi=0\ , \tag{2a}$$

where

$$t_2(S)\equiv p_2^{\,2}(S)=2E-[l(l+1)\hbar^2/S^2]\ . \tag{2b}$$

From a recent publication[6] we can see that, to order $\hbar^2$ (with corrections in the errors in signs),

$$\int_{S_1}^{S}p_2dS+\frac{\hbar^2}{24}\left(\int_{S_1}^{S}\frac{t_2''^{2}}{t_2^{1/2}t_2'^{2}}\,dS-\int_{S_1}^{S}\frac{t_2'''}{t_2^{1/2}t_2'}\,dS\right)=\int_{r_1}^{r}p_1dr+\frac{\hbar^2}{24}\left(\int_{r_1}^{r}\frac{t_1''^{2}}{t_1^{1/2}t_1'^{2}}\,dr-\int_{r_1}^{r}\frac{t_1'''}{t_1^{1/2}t_1'}\,dr\right), \tag{3}$$

where the assumption is made that, in intervals $S_1<S$ and $r_1<r$, $t_2(S_1)=0$, $t_1(r_1)=0$, $t_2'(S)\neq 0$, and $t_1'(r)\neq 0$. What we want to show in this paper is that we could extend Eq. (3) to include $\hbar^4$ terms and obtain further improvements as shown in Table I. In Ref. 6, we obtained the phase-integral for-

mula to order $\hbar^4$. However, in that paper the $\hbar^4$ terms of the phase integrals are given in terms of the contour integral in a complex plane such that the derivation is based upon a simplification, namely, by means, of the free wave functions. In the present problem we rewrite the phase integrals in terms of definite integrals. It is then applied to $1/r^4$ potential. The algebra becomes very complicated as we go to higher orders. By transforming the contour integrals into the ordinary definite integrals along the real axis only (Sec. II) we obtain the correct improvement at the low-energy limit. Here we think that it would be a straightforward job to write out the higher-order terms, and although it may be messy, we do not foresee any difficulty in using the same method.

II. GENERAL WKB PERTURBATION FORMULA EXPANDED TO ORDER $\hbar^4$ FOR ONE-TURNING-POINT SCATTERING CASE

The phase-integral formula as expanded to order $\hbar^4$ for the one-turning-point scattering case is

$$I_1+I_2=J_1+J_2\ , \tag{4a}$$

with

$$I_1=\int_{r_1}^{r} p_1 dr+\frac{\hbar^2}{24}\left(\int_{r_1}^{r}\frac{t_1''^2}{t_1^{1/2}t_1'^2}\,dr-\int_{r_1}^{r}\frac{t_1'''}{t_1^{1/2}t_1'}\,dr\right)\ , \tag{4b}$$

$$\begin{aligned}I_2=\frac{\hbar^4}{2880}\Bigg(&5\int_{r_1}^{r}\frac{t_1^{(\mathrm{vi})}}{t_1^{1/2}t_1'^2}\,dr-29\int_{r_1}^{r}\frac{t_1^{(\mathrm{v})}t_1'''}{t_1^{1/2}t_1'^3}\,dr-47\int_{r_1}^{r}\frac{t_1^{(\mathrm{iv})}t_1'''}{t_1^{1/2}t_1'^3}\,dr+140\int_{r_1}^{r}\frac{t_1''t_1'''^2}{t_1^{1/2}t_1'^4}dr\\&-106\int_{r_1}^{r}\frac{t_1''^2t_1^{(\mathrm{iv})}}{t_1^{1/2}t_1'^5}\,dr-280\int_{r_1}^{r}\frac{t_1''^3t_1'''}{t_1^{1/2}t_1'^5}\,dr+105\int_{r_1}^{r}\frac{t_1''^5}{t_1^{1/2}t_1'^6}\,dr\Bigg)\end{aligned} \tag{4c}$$

and with S replacing r, S_1 replacing r_1, and p_2 and t_2 replacing p_1 and t_1 respectively in the right-hand side for J_1 and J_2, where the Roman numerals inside the bracket indicate the number of times the function has been differentiated; for example

$$t^{(\mathrm{v})}=\frac{d^5t}{dr^5}\ .$$

Notice that the integrals involved are real and with $t_1(r_1)=0$ and $t_2(S_1)=0$, and $t_1'(r)\neq0$, $t_2'(S)\neq0$ for $r\geq r_1$ and $S\geq S_1$, so we see that all integrals are convergent. Equation (3) is expanded to include $\hbar^2$ terms and Eq. (4) is expanded to include $\hbar^4$ terms, which will give us the relationship between phase shifts. For short-range forces we have at large r and S

$$\psi(r)\simeq\sin(Kr-\tfrac{1}{2}L\pi+\delta_r)$$

and

$$\phi(S)\simeq\sin(KS-\tfrac{1}{2}\pi+\delta_S)\ ,$$

with $\hbar^2K^2=2E$. However, Eqs. (4) contain a relation between r and S. We can see, therefore, that

$$\lim_{\substack{r\to\infty\\ S\to\infty}}K(r-S)=\delta_S-\delta_r\ . \tag{5}$$

Here we set $\delta_S=0$, for we will use the three-dimensional free particle as the known case to be studied in the latter part.

The derivation of Eq. (4c) starts from Eq. (23) of Ref. 6. By using the formula $\oint udv=-\oint vdu$ several times, we see that

$$\begin{aligned}I_2&=-\frac{\hbar^4}{64}\oint p_1''^2p_1^{-5}dr+\hbar^4\tfrac{15}{256}\oint p_1'^4p_1^{-7}dr\\&=-\frac{\hbar^4}{3072}\oint t_1^{-7/2}t_1''^2dr+\frac{\hbar^4}{3072}\oint t_1^{-7/2}t_1't_1'''\,dr\\&=-\frac{\hbar^4}{5760}\Bigg[-7\oint t_1^{-1/2}\left(\frac{2t_1''t_1^{(\mathrm{v})}+6t_1'''t_1^{(\mathrm{iv})}}{t_1'^3}-\frac{20t_1''t_1'''^2+13t_1''^2t^{(\mathrm{iv})}}{t'^4}+\frac{40t_1''^3t_1'''}{t_1'^5}-\frac{15t_1''^5}{t_1'^6}\right)dr\\&\qquad+5\oint t_1^{-1/2}\left(\frac{t_1^{(\mathrm{vi})}}{t_1'^2}-\frac{3t_1^{(\mathrm{v})}t_1''}{t_1'^3}-\frac{t_1^{(\mathrm{iv})}t_1'''}{t_1'^3}+\frac{3t_1^{(\mathrm{iv})}t_1''^2}{t_1'^4}\right)dr\Bigg]\ ,\end{aligned} \tag{6}$$

where the integrations are around a closed contour above and below the real axis, with $r=r_1$ and $r=\infty$ included as previously specified. We can open the above contour integral since there are no divergences inside the integral now. So, after rearranging we get Eq. (4c).

III. LOW-ENERGY AND SMALL-COUPLING-CONSTANT PHASE SHIFTS OF THE REPULSIVE INVERSE-FOURTH-POWER POTENTIAL

We are presenting our results in the low-energy and small-coupling-constant limit. There is no difficulty in writing out the phase shifts in general terms where the energy and the coupling constant are not small. But we are interested in establishing the validity of the high-order terms like Eq. (4c), so we are concentrating our efforts in the low-energy, small-coupling-constant limit. What we are going to do here is to present the results first in Table I. (We list the contribution to eight decimal places.) This is essential, for then we can believe that the correction is in the right direction as well as of the right magnitude. The interesting thing that we have encountered is the fact that many terms in Eqs. (4) add up to such a small coefficient with the correct magnitude, as will be shown. So we believe that the $\hbar^4$ terms as given are essentially correct.

Since the terms to the order of $\hbar^2$ have already been reported in Ref. 1, we concentrate on the calculation of the $\hbar^4$ terms. To order $\hbar^2$, we have, instead of Eq. (3),

$$\begin{aligned}\lim_{\substack{S\to\infty\\ r\to\infty}} K(S-r) &= [l(l+1)]^{1/2}\tfrac{1}{2}\pi + \frac{1}{[l(l+1)]^{1/2}}\tfrac{1}{16}\pi \\ &\quad + (r_1^2+r_2^2)^{1/2}[-2E(\tfrac{1}{2}\pi, k) + F(\tfrac{1}{2}\pi, k)] \\ &\quad - \frac{1}{24K}\left\{ \frac{3F(\tfrac{1}{2}\pi, k)}{(r_1^2+r_2^2)^{1/2}} + 6r_3^2 A_1 - \frac{64g^4 A_2}{\hbar^2[l(l+1)]^2} \right\} , \qquad (7)\end{aligned}$$

where

$$r_1^2 = (1/2K^2)(l(l+1) + \{[l(l+1)]^2 + 8g^2K^2/\hbar^2\}^{1/2}),$$

$$r_2^2 = (-1/2K^2)(l(l+1) - \{[l(l+1)]^2 + 8g^2K^2/\hbar^2\}^{1/2}),$$

$$k^2 = r_2^2/(r_1^2+r_2^2) ,$$

$$r_3^2 = 4g^2/[l(l+1)]\hbar^2 ,$$

$$A_1 = \int_{r_1}^{r} \frac{dr}{[(r^2-r_1^2)(r^2+r^2)]^{1/2}(r^2+r_3^2)} ,$$

and

$$A_2 = \int_{r_1}^{r} \frac{dr}{[(r^2-r_1^2)(r^2+r_2^2)]^{1/2}(r^2+r_3^2)^2} .$$

Of course if g is set to zero, Eq. (7) should be an identity except that S is replaced by r. Equation (7) further reduces to

$$\begin{aligned}\delta_l^{(1)} &= \lim_{\substack{S\to\infty\\ r\to\infty}} K(r-S) \\ &= \{K^2 g^2 \tfrac{1}{4}\pi[l(l+1)]^{3/2}\}\left[1 + \frac{5}{8l(l+1)}\right] \qquad (8)\end{aligned}$$

TABLE I. A list of S_1, S_2, S_3, and S_4 as defined by the following relationships: The exact phase shifts are $\delta_l = 2\pi K^2 g^2 S_1$, the phase shifts to zeroth order in $\hbar^2$ are $\delta_l^{(0)} = 2\pi K^2 g^2 S_2$, the phase shifts to first order in $\hbar^2$ are $\delta_l^{(1)} = 2\pi K^2 g^2 S_3$, and the phase shifts to second order in $\hbar^2$ are $\delta_l^{(2)} = 2\pi K^2 g^2 S_4$. Remember that all of these values are an approximation to first order in $K^2 g^2$. $S_1 = 1/(2l+1)(2l-1)(2l+3)$, $S_2 = 1/8[l(l+1)]^{3/2}$, $S_3 = S_2[1+5/8l(l+1)]$, and $S_4 = S_2(1+5/8l(l+1) + 0.49\{1/[l(l+1)]^2\})$.

l	S_1	S_2	S_3	S_4
1	0.066 666 67	0.044 194 17	0.058 004 85	0.063 418 64
2	0.009 523 81	0.008 505 17	0.009 391 13	0.009 506 89
3	0.003 174 60	0.003 007 03	0.003 163 65	0.003 173 88
4	0.001 443 00	0.001 397 54	0.001 441 22	0.001 442 93
5	0.000 777 00	0.000 760 73	0.000 776 57	0.000 776 99
6	0.000 466 20	0.000 459 24	0.000 466 07	0.000 466 20

if we keep only terms to order $K^2 g^2$.

We will obtain the higher-order, or order-$\hbar^4$, contribution. The trick here is to first perform the integrations in terms of elliptic functions and then find the corresponding expansions for the elliptic functions. We obtain, therefore,

$$\lim_{\substack{r\to\infty\\ g^2K^2\to 0}} \int_{r_1}^{r} \frac{t_1^{(vi)}}{t_1^{1/2} t_1'^2}\, dr = -\frac{1260}{l(l+1)\hbar^3 K} B_1 - \frac{7560 g^2 K^2 \pi}{[l(l+1)]^{7/2}\hbar^5} , \qquad (9a)$$

$$\lim_{\substack{r\to\infty\\ g^2K^2\to 0}} \int_{r_1}^{r} \frac{t_1^{(v)} t_1''}{t_1^{1/2} t_1'^3}\, dr = -\frac{540}{l(l+1)\hbar^3 K} B_2 - \frac{3420 g^2 K^2 \pi}{[l(l+1)]^{7/2}\hbar^5} , \qquad (9b)$$

$$\lim_{\substack{r\to\infty\\ g^2K^2\to 0}} \int_{r_1}^{r} \frac{t_1^{(iv)} t_1'''}{t_1^{1/2} t_1'^3}\, dr = -\frac{360}{l(l+1)\hbar^3 K} B_2 - \frac{2160 g^2 K^2 \pi}{[l(l+1)]^{7/2}\hbar^5} , \qquad (9c)$$

$$\lim_{\substack{r\to\infty\\ g^2K^2\to 0}} \int_{r_1}^{r} \frac{t_1'' t_1'''^2}{t_1^{1/2} t_1'^4}\, dr = -\frac{216}{l(l+1)\hbar^3 K} B_3 - \frac{792 g^2 K^2 \pi}{[l(l+1)]^{7/2}\hbar^5} , \qquad (9d)$$

$$\lim_{\substack{r\to\infty\\ g^2K^2\to 0}} \int_{r_1}^{r} \frac{t_1''^2 t_1^{(iv)}}{t_1^{1/2} t_1'^5}\, dr = -\frac{270}{l(l+1)\hbar^3 K} B_3 - \frac{1035 g^2 K^2 \pi}{[l(l+1)]^{7/2}\hbar^5} , \qquad (9e)$$

$$\lim_{\substack{r\to\infty\\ g^2K^2\to 0}} \int_{r_1}^{r} \frac{t_1''^3 t_1'''}{t_1^{1/2} t_1'^5}\, dr = -\frac{162}{l(l+1)\hbar^3 K} B_3 - \frac{567 g^2 K^2 \pi}{[l(l+1)]^{7/2}\hbar^5} , \qquad (9f)$$

and

$$\lim_{\substack{r\to\infty \\ g^2K^2\to 0}} \int_{r_1}^{r} \frac{t_1''^5}{t_1^{1/2} t_1'^6}\, dr = -\frac{243}{2l(l+1)\hbar^3 K} B_3 - \frac{405 g^2 K^2 \pi}{[l(l+1)]^{7/2}\hbar^5}, \tag{9g}$$

where

$$B_1 \equiv \lim_{\substack{r\to\infty \\ g^2K^2\to 0}} \int_{r_1}^{r} \frac{r^4 dr}{[(r^2 - r_1^2)(r^2 + r_2^2)]^{1/2}(r^2 + r_3^2)^2} = \frac{\pi K}{2[l(l+1)]^{1/2}} \left\{1 - \frac{11}{2}\frac{g^2K^2}{[l(l+1)]^2\hbar^2}\right\},$$

$$B_2 \equiv \lim_{\substack{r\to\infty \\ g^2K^2\to 0}} \int_{r_1}^{r} \frac{r^6 dr}{[(r^2 - r_1^2)(r^2 + r_2^2)]^{1/2}(r^2 + r_3^2)^3} = \frac{\pi K}{2[l(l+1)]^{1/2}} \left\{1 - \frac{15}{2}\frac{g^2K^2}{[l(l+1)]^2\hbar^2}\right\},$$

and

$$B_3 \equiv \lim_{\substack{r\to\infty \\ g^2K^2\to 0}} \int_{r_1}^{r} \frac{r^2 dr}{[(r^2 - r_1^2)(r^2 + r_2^2)]^{1/2}(r^2 + r_3^2)} = \frac{\pi K}{2[l(l+1)]^{1/2}} \left\{1 - \frac{7}{4}\frac{g^2K^2}{[l(l+1)]^2\hbar^2}\right\}.$$

Substituting Eqs. (9a)–(9g) into Eq. (4), we obtain to the order of $\hbar^4$ and to the order of K^2g^2 the expression

$$\delta_l^{(2)} = \lim_{\substack{S\to\infty \\ r\to\infty}} K(r - S) = \{K^2 g^2 \tfrac{1}{4}\pi [l(l+1)]^{3/2}\} \times \left\{1 + \frac{5}{8l(l+1)} + 0.49\frac{1}{[l(l+1)]^2}\right\}. \tag{10}$$

From Table I, we see that Eq. (10) yields a δ_l which is a closer approximation than was given before by Eq. (8).

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