Phase shifts due to a mixture of long- and short-range potentials

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We show that the generalized or modified WKB method can be readily applied to a mixture of long- and short-range potentials. The phase shifts of such a mixed potential are calculated to order $\hbar^2$ by using the solutions of the long-range potential as the bases of the approximation and treating the differences between the long-range and mixed potential as a WKB perturbation. We demonstrate the method by a simple example using a Coulomb and inverse-square potential. Comparison of the phase shifts with the exact results shows excellent agreement. The phase shifts can then be separated into contributions due to the long-range and short-range potentials plus a contribution due to the mixture or coupling of the potentials. For small angular momenta, the contribution due to coupling is of the same order of magnitude as the Coulomb contribution, but rapidly decreases with higher angular momentum.

I. INTRODUCTION

In recent years, the measurements in scattering experiments have become more exact. In many cases, the potential that one encounters consists of a mixture of long- and short-range potentials. The conventional WKB treatment cannot be applied to such a mixed potential. Vollmer[1] pointed this out in his WKB treatment of the inversion problem. In treating mixed potentials of this type, one can truncate the long-range potential at some finite distance[2] or apply a distorted-wave Born approximation. The generalized WKB (GWKB) method offers another alternative. The attractive feature of the GWKB method is that it remains valid in the low-energy region. Since the conventional WKB approximation is a special case of the generalized WKB approximation, the GWKB treatment can be readily applied to a greater variety of problems over a larger range of energies.

Applying the GWKB method to a pure long-range potential, one of us[3] was able to obtain the specific Coulomb phase shifts to order $\hbar^2$ which agreed with the results given by Rosen and Yennie.[4] However, no consideration was given to the problem of long- and short-range potentials. We now address ourselves to this problem in order to extend the usefulness of the GWKB method.

In applying the GWKB method,[5] one formulates a model potential that is qualitatively similar to the actual potential and whose Schrödinger equation can be solved exactly. Using the exact solutions of the model as the bases of the approximation, one can obtain an approximation of the wave functions for the actual potential. The differences between the actual and model potential can then be treated as a WKB perturbation. Since the long-range potential is dominant at large distances, it is a logical choice for the model potential. One then determines the phase-shift difference between model and actual potential (which in this case consists of a short-range potential plus the long-range potential). The total phase shift for the mixed potential can then be obtained by adding the phase shift of the long-range potential to this difference. In Sec. II, the GWKB method is applied to a mixed potential which is made up of an arbitrary long- and short-range potential. The approximation to zeroth and first order in $\hbar^2$ along with the phase-shift connection formula is presented. Using a Coulomb and inverse-square potential as a simple example in Sec. III, we calculate the zeroth- and first-order phase shifts in order to demonstrate the contribution of the higher-order terms to the approximation. Comparison of the phase shifts with the exact results, as presented in Table I, shows excellent agreement.

The expression for the phase shifts can then be separated and identified as contributions due to the Coulomb and inverse-square potentials plus a contribution due to the mixing or coupling of the two potentials. The results are presented in Table II.

II. METHOD OF APPROXIMATION

In general, we wish to solve the radial Schrödinger equation

$$\left(\frac{d^2}{dr^2}+\frac{P_1^2(r)}{\hbar^2}\right)\psi_l(r)=0\,, \tag{1}$$

where

$$\begin{aligned}\psi_l(r)&=rR_l(r)\,,\\ P_1^2(r)&=t_1(r)\\ &=\left(k^2-\frac{2\mu}{\hbar^2}\left[V_{\text{l.r.}}(r)+V_{\text{s.r.}}(r)\right]-\frac{\alpha}{r^2}\right),\\ \alpha&=l(l+1)\,.\end{aligned} \tag{2}$$

The long-range and short-range potentials are

TABLE I. Phase shifts due to Coulomb and inverse-square potentials. (a) GWKB approximation to zeroth order in $\hbar^2$, (b) GWKB approximation to first order in $\hbar^2$, (c) exact results as given by Eq. (21).

k	η	$2\mu V_0^{\text{s.r.}}/\hbar^2$	β	l	(a)	(b)	(c)
2	0.250	4	6	1	−1.3831	−1.3380	−1.3398
2	0.250	6	12	2	−1.2763	−1.2563	−1.2566
2	0.250	8	20	3	−1.2055	−1.1941	−1.1942
2	0.250	10	30	4	−1.1515	−1.1442	−1.1442
2	0.250	12	42	5	−1.1077	−1.1025	−1.1025
4	−0.125	4	6	1	−1.7477	−1.6821	−1.6862
4	−0.125	6	12	2	−1.7524	−1.7272	−1.7278
4	−0.125	8	20	3	−1.7724	−1.7589	−1.7591
4	−0.125	10	30	4	−1.7924	−1.7840	−1.7841
4	−0.125	12	42	5	−1.8106	−1.8049	−1.8049
2	−0.250	−4	2	2	1.5316	1.4594	1.4641
2	−0.250	−6	6	3	1.3660	1.3391	1.3398
2	−0.250	−8	12	4	1.2706	1.2564	1.2566
2	−0.250	−10	20	5	1.2028	1.1941	1.1942
2	−0.250	−12	30	6	1.1501	1.1442	1.1442
4	0.125	−4	2	2	1.6730	1.6213	1.6238
4	0.125	−6	6	3	1.7075	1.6857	1.6862
4	0.125	−8	12	4	1.7398	1.7277	1.7278
4	0.125	−10	20	5	1.7667	1.7590	1.7591
4	0.125	−12	30	6	1.7894	1.7841	1.7841

defined by

$$\lim_{r\to\infty} rV_{\text{l.r.}}(r) = b\,,$$

$$\lim_{r\to\infty} rV_{\text{s.r.}}(r) = 0\,,$$

where b is a nonzero constant.

Selecting the long-range potential as the model potential whose Schrödinger equation can be solved exactly, we have

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

where

$$\begin{aligned}\phi_l(s) &= sR_l(s)\,,\\ P_2^{\,2}(s) &= t_2(s)\\ &= \left(k^2-\frac{2\mu}{\hbar^2}V_{\text{l.r.}}(s)-\frac{\alpha}{s^2}\right),\\ \alpha &= l(l+1)\,,\end{aligned} \tag{4}$$

and the phase shifts, $\sigma_{\text{l.r.}}$, are known. As a special case, the generalized WKB method reduces to the conventional WKB method when $P_2(s)=1$.

Now the solution of Eqs. (1) and (3) must be of the form

TABLE II. Contributions to the total phase shifts for $2\mu V_0^{\text{s.r.}}/\hbar^2=10$ and $\mu z e^2/\hbar^2=-1$.

k	l	σ_c	$\sigma_{\text{s.r.}}$	γ	γ/σ_c
2	1	−0.2189	−3.1378	−0.4072	1.8602
	2	−0.4641	−2.4045	−0.2346	0.5055
	3	−0.6294	−1.9115	−0.1477	0.2347
	4	−0.7538	−1.5707	−0.0997	0.1323
	5	−0.8535	−1.3262	−0.0711	0.0833
	6	−0.9370	−1.1442	−0.0529	0.0565
10	1	−0.0423	−3.1378	−0.0826	1.9527
	2	−0.0923	−2.4045	−0.0473	0.5125
	3	−0.1256	−1.9115	−0.0297	0.2365
	4	−0.1506	−1.5707	−0.0200	0.1328
	5	−0.1706	−1.3262	−0.0142	0.0832
	6	−0.1873	−1.1442	−0.0106	0.0566
20	1	−0.0212	−3.1378	−0.0413	1.9481
	2	−0.0461	−2.4045	−0.0237	0.5141
	3	−0.0628	−1.9115	−0.0148	0.2357
	4	−0.0753	−1.5707	−0.0100	0.1328
	5	−0.0853	−1.3262	−0.0071	0.0832
	6	−0.0936	−1.1442	−0.0053	0.0566
30	1	−0.0141	−3.1378	−0.0275	1.9504
	2	−0.0308	−2.4045	−0.0158	0.5130
	3	−0.0419	−1.9115	−0.0099	0.2363
	4	−0.0502	−1.5707	−0.0067	0.1335
	5	−0.0569	−1.3262	−0.0047	0.0826
	6	−0.0624	−1.1442	−0.0035	0.0561

$$\psi_l(r) \underset{r\to\infty}{\sim} \sin[kr+f(kr)-\tfrac{1}{2}\pi l+\delta_l]\,,$$

$$\phi_l(s) \underset{s\to\infty}{\sim} \sin[ks+f(ks)-\tfrac{1}{2}\pi l+\sigma_{\text{l.r.}}]\,,$$

so that the phase shifts of the model are connected to the phase shifts of the actual problem by

$$\delta_l-\sigma_{\text{l.r.}}=\lim_{r\to\infty}[ks-kr+f(ks)-f(kr)]\,, \tag{5}$$

which is the phase-shift difference. Equation (5) is the phase-shift connection formula.

To zeroth order in $\hbar^2$, the model is connected to the actual problem by the phase integrals[5]

$$\int_{s_1}^{s} P_2(s)ds=\int_{r_1}^{r} P_1(r)dr\,, \tag{6}$$

where s is defined to be a function of r, and s_1 and r_1 are the classical turning points of the model and actual problem which satisfies the condition $P_2(s_1)=P_1(r_1)=0$. Therefore,

$$\lim_{r\to\infty}[ks-kr+f(ks)-f(kr)] =\lim_{r\to\infty}\left(\int_{s_1}^{s} P_2(s)ds-\int_{r_1}^{r} P_1(r)dr\right). \tag{7}$$

To first order in $\hbar^2$, the phase-integral relationship is given by (See Ref. 6 for details)

$$\int_{s_1}^{s} P_2(s)ds + \frac{\hbar^2}{12}\int_{s_1}^{s} G(t_2)t_2^{1/2}(s)ds = \int_{r_1}^{r} P_1(r)dr + \frac{\hbar^2}{12}\int_{r_1}^{r} G(t_1)t_1^{1/2}(r)dr\,, \quad (8)$$

where

$$G(t_i) = \frac{t_i''''}{t_i'^2} - 4\frac{t_i'''t_i''}{t_i'^3} + 3\frac{t_i''^3}{t_i'^4}\,, \quad (9)$$

and the primes indicate differentiation. Therefore,

$$\lim_{r\to\infty}[ks - kr + f(ks) - f(kr)] = \lim_{r\to\infty}\left[\int_{s_1}^{s} P_2(s)ds - \int_{r_1}^{r} P_1(r)dr + \frac{\hbar^2}{12}\int_{s_1}^{s} G(t_2)t_2^{1/2}(s)ds - \frac{\hbar}{12}\int_{r_1}^{r} G(t_1)t_1^{1/2}(r)dr\right], \quad (10)$$

so that the phase shifts of the actual potential are given by

$$\delta_l = \sigma_{\text{l.r.}} + \lim_{r\to\infty}[ks - kr + f(ks) - f(kr)]\,. \quad (11)$$

III. APPLICATION TO A COULOMB AND INVERSE-SQUARE POTENTIAL

In this section, we choose a Coulomb and inverse-square potential as an example. The selection of the inverse-square potential as the short-range potential was based upon the desirability of presenting a simple example that clearly illustrates the GWKB method and allows for a simple verification of the results.

The long-and short-range potentials are then given by

$$V_{\text{l.r.}}(r) = Ze^2/r\,,$$

$$V_{\text{s.r.}}(r) = V_0^{\text{s.r.}}/r^2\,,$$

and the Schrödinger equation becomes

$$\left[\frac{d^2}{d\rho^2} + \frac{P_1^2(\rho)}{\hbar^2}\right]\psi_l(\rho) = 0\,, \quad (12)$$

where

$$\begin{aligned} &\rho = kr\,,\\ &P_1^2(\rho) = t_1(\rho)\\ &\qquad = \hbar^2\left(1 - \frac{2\eta}{\rho} - \frac{\beta}{\rho^2}\right),\\ &\eta = \frac{\mu Ze^2}{\hbar^2 k}\,,\\ &\beta = \frac{2\mu V_0^{\text{s.r.}}}{\hbar^2} + \alpha\,,\\ &\alpha = l(l+1)\,. \end{aligned} \quad (13)$$

The model equation is given by

$$\left(\frac{d^2}{dv^2} + \frac{P_2^2(v)}{\hbar^2}\right)\phi_l(v) = 0\,, \quad (14)$$

where

$$\begin{aligned} &v = ks\,,\\ &P_2^2(v) = t_2(v)\\ &\qquad = \hbar^2\left(1 - \frac{2\eta}{v} - \frac{\alpha}{v^2}\right),\\ &\alpha = l(l+1)\,. \end{aligned} \quad (15)$$

The phase shifts for the Coulomb potential are given by

$$\sigma_c = \arg\Gamma(l+1+i\eta) = \eta\psi(l+1) + \sum_{k=0}^{\infty}\left(\frac{\eta}{k+l+1} - \tan^{-1}\frac{\eta}{k+l+1}\right). \quad (16)$$

The classical turning points are given by the condition $P_l(v_1) = P_1(\rho_1) = 0$, so that

$$v_1 = \eta + (\eta^2 + \alpha)^{1/2}\,,$$

$$\rho_1 = \eta + (\eta^2 + \beta)^{1/2}\,,$$

and the phase-integral relationship to zeroth order in $\hbar^2$, given by Eq. (6), can be written as

$$\int_{v_1}^{v}(v^2 - 2\eta v - \alpha)^{1/2}\frac{dv}{v} = \int_{\rho_1}^{\rho}(\rho^2 - 2\eta\rho - \beta)^{1/2}\frac{d\rho}{\rho}\,,$$

and Eq. (7) becomes

$$\lim_{\rho\to\infty}\left(v - \rho - \eta\ln\frac{v}{\rho}\right) = \tfrac{1}{2}\eta\ln\left(\frac{\eta^2+\beta}{\eta^2+\alpha}\right) + \beta^{1/2}\sin^{-1}\left(\frac{\eta}{(\eta^2+\beta)^{1/2}}\right) - \alpha^{1/2}\sin^{-1}\left(\frac{\eta}{(\eta^2+\alpha)^{1/2}}\right) - \frac{\pi}{2}(\beta^{1/2} - \alpha^{1/2})\,. \quad (17)$$

To zeroth order in $\hbar^2$, Eq. (11) becomes

$$\delta_l^{\text{GWKB}} = \sigma_c + \tfrac{1}{2}\eta\ln\left(\frac{\eta^2+\beta}{\eta^2+\alpha}\right) + \beta^{1/2}\sin^{-1}\left(\frac{\eta}{(\eta^2+\beta)^{1/2}}\right) - \alpha^{1/2}\sin^{-1}\left(\frac{\eta}{(\eta^2+\alpha)^{1/2}}\right), \quad (18)$$

where σ_c is given by Eq. (16).

Substituting Eqs. (13) and (15) into Eq. (9) yields

$$G(t_1)=\frac{3\beta^2(2\eta\rho+\beta)}{2\hbar^2(\eta\rho+\beta)^4},\quad G(t_2)=\frac{3\alpha^2(2\eta v+\alpha)}{2\hbar^2(\eta v+\alpha)^4},$$

so that Eq. (10) becomes

$$\lim_{\substack{\rho\to\infty\\ v\to\infty}}\left(v-\rho-\eta\ln\frac{v}{\rho}\right)=\tfrac{1}{2}\eta\ln\left(\frac{\eta^2+\beta}{\eta^2+\alpha}\right)+\left(\beta^{1/2}+\frac{1}{8\beta^{1/2}}\right)\sin^{-1}\left(\frac{\eta}{(\eta^2+\beta)^{1/2}}\right)-\left(\alpha^{1/2}+\frac{1}{8\alpha^{1/2}}\right)\sin^{-1}\left(\frac{1}{(\eta^2+\alpha)^{1/2}}\right)$$
$$-\frac{\pi}{2}(\beta^{1/2}-\alpha^{1/2})-\frac{\pi}{16}\left(\frac{1}{\beta^{1/2}}-\frac{1}{\alpha^{1/2}}\right)-\frac{\eta(\beta-\alpha)}{24(\eta^2+\beta)(\eta^2+\alpha)}. \tag{19}$$

The phase shifts to first order in $\hbar^2$ are given by

$$\delta_l^{\rm GWKB}=\sigma_c-\left(\beta^{1/2}+\frac{1}{8\beta^{1/2}}-\alpha^{1/2}-\frac{1}{8\alpha^{1/2}}\right)\frac{\pi}{2}+\tfrac{1}{2}\eta\ln\left(\frac{\eta^2+\beta}{\eta^2+\alpha}\right)+\left(\beta^{1/2}+\frac{1}{8\beta^{1/2}}\right)\sin^{-1}\left(\frac{\eta}{(\eta^2+\beta)^{1/2}}\right)$$
$$-\left(\alpha^{1/2}-\frac{1}{8\alpha^{1/2}}\right)\sin^{-1}\left(\frac{\eta}{(\eta^2+\alpha)^{1/2}}\right)-\frac{\eta(\beta-\alpha)}{24(\eta^2+\beta)(\eta^2+\alpha)}, \tag{20}$$

where σ_c is given by Eq. (16).

The validity of Eqs. (18) and (20) can be easily verified by allowing $2\mu V_0^{\rm s.r.}/\hbar^2$ to take on integer values such that

$$\beta=\frac{2\mu V_0^{\rm s.r.}}{\hbar^2}+l(l+1)$$
$$=L(L+1)$$
$$=\begin{cases}(l+1)(l+2)\\ l(l-1)\end{cases}$$

for

$$\frac{2\mu V_0^{\rm s.r.}}{\hbar^2}=\begin{cases}2l+2\\ -2l\end{cases}.$$

This approach is mainly for convenience so that

$$\delta_{\rm exact}=\arg\Gamma((l\pm1)+1+i\eta)\mp\tfrac{1}{2}\pi. \tag{21}$$

The results of Eqs. (18), (20), and (21) are presented in Table I and show excellent agreement. Comparing the zeroth- and first-order phase shifts with the exact results shows that inclusion of the higher-order terms improves the accuracy of the approximation.

The phase shifts to first order in $\hbar^2$, given by Eq. (20), can be rewritten in the form

$$\delta_l^{\rm GWKB}=\sigma_c+\sigma_{\rm s.r.}+\gamma, \tag{22}$$

where

$$\sigma_{\rm s.r.}=\left(\alpha^{1/2}+\frac{1}{8\alpha^{1/2}}-\beta^{1/2}-\frac{1}{8\beta^{1/2}}\right)\frac{\pi}{2}, \tag{23}$$

$$\gamma=\tfrac{1}{2}\eta\ln\left(\frac{\eta^2+\beta}{\eta^2+\alpha}\right)+\left(\beta^{1/2}+\frac{1}{8\beta^{1/2}}\right)\sin^{-1}\left(\frac{\eta}{(\eta^2+\beta)^{1/2}}\right)$$
$$-\left(\alpha^{1/2}+\frac{1}{8\alpha^{1/2}}\right)\sin^{-1}\left(\frac{\eta}{(\eta^2+\alpha)^{1/2}}\right)$$
$$-\frac{\eta(\beta-\alpha)}{24(\eta^2+\beta)(\eta^2+\alpha)}, \tag{24}$$

and σ_c is given by Eq. (16). $\sigma_{\rm s.r.}$ can be easily identified as the short-range contribution to the phase shift by merely setting $\eta=0$ or solving for the phase shifts due to a pure inverse-square potential. Since γ vanishes when either potential is "turned off," e.g., $\eta=0$ or $\beta=\alpha$, it can be lossely interpreted as a coupling term due to the mixing of the two potentials. Because of the particular nature of the inverse-square potential, the phase-shift contribution ($\sigma_{\rm s.r.}$) is independent of energy. In general, the short-range phase-shift contribution will be energy dependent and should decrease with higher energy. Because $\sigma_{\rm s.r.}$ is independent of energy in this case, a comparison can be made between γ and σ_c, and the results are presented in Table II. For small angular momenta, γ is of the same order of magnitude as σ_c and cannot be ignored. However, γ decreases rapidly with increasing values of l, so that

$$\delta_l\simeq\sigma_c+\sigma_{\rm s.r.}$$

may prove to be a good approximation for the phase shifts due to a mixture of long- and short-range potentials outside the low-energy small-l region.

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