Inversion problem including a long-ranged potential in the generalized WKB method

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The generalized WKB method is applied to the construction of a potential which has a Coulomb tail. A simple numerical example is used to illustrate the accuracy of the terms to the order $\hbar^2$.

I. INTRODUCTION

The conventional WKB method is only applicable to the inversion of scattering phase shifts due to a short-ranged potential $V(r)$ [$\lim_{r\to\infty} rV(r)=0$]. Because of this constraint, one is confined to the inversion of molecular scattering data.[1] When Coulomb scattering is involved, the conventional WKB approximation is no longer applicable. It was shown by Wald *et al.*[2] that the generalized WKB method (Miller and Good[3]) can be used to construct a potential which has short-ranged and long-ranged parts. The appropriate formulas correct to the zeroth order of $\hbar^2$ were also derived. Terms to the order of $\hbar^2$ were derived by Vasilevsky *et al.*[4]

The inversion problem is to identify this potential $V(r)$ by means of a group of phase shifts. We see that, therefore, it needs high accuracy, and the WKB approximation to a higher order in $\hbar^2$ provides such accuracy. In the next section, the integral Abelian equation is derived in the zeroth-order approximation. We show explicitly that the constraint $\lim_{r\to\infty} rV(r)=0$ is replaced by $\lim_{r\to\infty}[rV(r)-rW(r)]=0$, where $W(r)$ is the model potential. In Sec. III, we derive the integral equation of the higher-order correction from a phase-integral equation developed in Ref. 5. Since the solutions of the above-mentioned integral equations are given in Vasilevsky *et al.*,[4] we just quote their results. In the last section, we present the numerical procedure and results in detail. It gives us confidence in this generalized WKB method. We see that the agreement in potential is very good indeed.

II. ZEROTH-ORDER APPROXIMATION IN $\hbar^2$

We start from the conventional WKB phase shift

$$\delta(E,l)=\sqrt{\lambda}\left[\int_{r_t}^{\infty} dr\left(E-U(r)-\frac{qE}{r^2}\right)^{1/2} - \int_{\sqrt{q}}^{\infty} dr\left(E-\frac{qE}{r^2}\right)^{1/2}\right], \tag{1}$$

where

$$q=\frac{l(l+1)}{\lambda E} \quad \text{and} \quad \lambda=\frac{2\mu}{\hbar^2}.$$

In the generalized WKB approximation, the generalization of (1) is

$$\delta(E,l)-\eta(E,l)=\sqrt{\lambda}\left[\int_{r_t}^{\infty} dr\left(E-U(r)-\frac{qE}{r^2}\right)^{1/2} - \int_{s_t}^{\infty} ds\left(E-W(s)-\frac{qE}{s^2}\right)^{1/2}\right], \tag{2}$$

where $\eta(E,l)$ is the phase shift of the model potential $W(s)$ and r_t, s_t are the turning points.

We define

$$U(r,l)=U(r)+\frac{qE}{r^2}, \qquad W(s,l)=W(s)+\frac{qE}{s^2}. \tag{3}$$

Integrating the integrals in (2) by parts, we have

$$\delta(E,l)-\eta(E,l)=\sqrt{\lambda}\left(\lim_{r\to\infty}\{r[E-U(r,l)]^{1/2}-r[E-W(r,l)]^{1/2}\} + \int_{r_t}^{\infty}\frac{1}{2}\frac{rU'(r,l)}{[E-U(r,l)]^{1/2}}dr - \int_{s_t}^{\infty}\frac{1}{2}\frac{sW'(s,l)}{[E-W(s,l)]^{1/2}}ds\right). \tag{4}$$

If $\lim_{r\to\infty}\{r[W(r)-U(r)]\}=0$, (3) becomes the following integral Abelian equation:

$$\int_{r_0}^{\infty}\frac{rU_0'(r,l)dr}{[E-U_0(r,l)]^{1/2}}=\frac{2}{\sqrt{\lambda}}[\delta(E,l)-\eta(E,l)]+\int_{s_t}^{\infty}\frac{sW'(s,l)ds}{[E-W(s,l)]^{1/2}}, \tag{5}$$

where the subscript 0 has been included to show that the approximation is of the zeroth order in $\hbar^2$.

The solution of (4) as given in Vasilevsky *et al.*[4] is written as

$$r(q_0)=s(q_0)\exp[M(q_0)], \tag{6}$$

$$U_0(r(q_0))=E[1-q_0/r^2(q_0)], \tag{7}$$

$$M(q_0)=\frac{2}{\pi(\lambda E)^{1/2}}\int_{q_0}^{\infty}\left(\frac{\partial\delta}{\partial q}-\frac{\partial\eta}{\partial q}\right)\frac{dq}{(q-q_0)^{1/2}}, \tag{8}$$

where $s(q_0)$ is the root of the equation

$$Eq_0=s^2[E-W(s)], \tag{9}$$

and q_0 is the parameter to be preset.

III. FIRST-ORDER APPROXIMATION IN $\hbar^2$

We start from the generalized phase-integral equation given in Ref. 5:

$$\oint p\,dr-\tfrac{1}{48}\hbar^2\oint\frac{t''\,dr}{t^{3/2}}=\oint P\,ds-\tfrac{1}{48}\hbar^2\oint\frac{T''ds}{T^{3/2}}, \tag{10}$$

where

$$t=p^2=2\mu[E-U(r,l)],$$

$$T=P^2=2\mu[E-W(s,l)].$$

Equation (10) can be rewritten as

$$\oint[E-U(r,l)]^{1/2}\,dr-\frac{1}{24}\left(\frac{\hbar^2}{2\mu}\right)\frac{\partial}{\partial E}\oint\frac{U''(r,l)dr}{[E-U(r,l)]^{1/2}}=\oint[E-W(s,l)]^{1/2}ds$$
$$-\frac{1}{24}\left(\frac{\hbar^2}{2\mu}\right)\frac{\partial}{\partial E}\oint\frac{W''(s,l)ds}{[E-W(s,l)]^{1/2}}. \tag{11}$$

Since $U(r)$ is the unknown in this case, we expand $U(r)$ as follows:

$$U(r)=U_0(r)+\hbar^2U_2(r). \tag{12}$$

Substituting (12) into (11) and collecting terms of the order of $\hbar^0$ and $\hbar^2$, respectively, we obtain

$$\oint[E-U_0(r,l)]^{1/2}=\oint[E-W(s,l)]^{1/2}, \tag{13}$$

$$\oint\frac{U_2(r)dr}{[E-U_0(r,l)]^{1/2}}=\frac{1}{12\lambda}\left(\frac{\partial}{\partial E}\oint\frac{W''(s,l)ds}{[E-W(s,l)]^{1/2}}-\frac{\partial}{\partial E}\oint\frac{U''(r,l)dr}{[E-U_0(r,l)]^{1/2}}\right). \tag{14}$$

The integrals in (14) are improper but convergent so they can be evaluated on the real axis. Therefore,

$$\int_{r_t}^{\infty}\frac{U_2(r)dr}{[E-U_0(r,l)]^{1/2}}=\frac{1}{12\lambda}\left(\frac{\partial}{\partial E}\int_{s_t}^{\infty}\frac{W''(s,l)ds}{[E-W(s,l)]^{1/2}}-\frac{\partial}{\partial E}\int_{r_t}^{\infty}\frac{U''(r,l)dr}{[E-U_0(r,l)]^{1/2}}\right). \tag{15}$$

The solution of (15) is given in Vasilevsky *et al.*[4] We just quote their result:

$$U_2(r(q_0))=\frac{1}{12\lambda}\left\{\left[\frac{r'''}{(r')^3}-\frac{2(r'')^2}{(r')^4}+\frac{r''}{r(r')^2}-\frac{3}{r^2}\right]-\left(\frac{ss'}{rr'}\right)\left[\frac{s'''}{(s')^3}-\frac{2(s'')^2}{(s')^4}+\frac{s''}{s(s')^2}-\frac{3}{s^2}\right]\right\}, \tag{16}$$

where the prime can be interpreted as $\partial/\partial q_0$ or $\partial/\partial(q_0E)$.

IV. NUMERICAL PROCEDURE

The simplest example is the inversion of phase shifts due to the scattering potential

$$U(r)=\frac{A}{r}+\frac{B}{r^2}. \tag{17}$$

As shown in Sec. I, we must choose the model potential $W(s)$ subject to the constraint $\lim_{r\to\infty}\{r[W(r)-U(r)]\}=0$. In this example, the obvious choice is

$$W(s)=\frac{A}{s}\ . \tag{18}$$

The phase shifts due to these potentials are well known. They are

$$\eta(E,l)=\arg\Gamma(l+1+iA/2\sqrt{E})-\tfrac{1}{2}l\pi\ , \tag{19}$$

$$\delta(E,l)=\arg\Gamma\left(\left[B+(l+\tfrac{1}{2})^2\right]^{1/2}+\tfrac{1}{2}+i\frac{A}{2\sqrt{E}}\right)+\tfrac{1}{2}\pi\left\{\tfrac{1}{2}-\left[B+(l+\tfrac{1}{2})^2\right]^{1/2}\right\}\ . \tag{20}$$

Setting $\hbar^2=2\mu=1$ and expressing l in terms of q, we obtain

$$\eta(E,q)=\arg\Gamma\left((\tfrac{1}{4}+qE)^{1/2}+\tfrac{1}{2}+iA/2\sqrt{E}\right)+\tfrac{1}{2}\pi\left[\tfrac{1}{2}-(B+\tfrac{1}{4}+qE)^{1/2}\right], \tag{21}$$

$$\delta(E,q)=\arg\Gamma\left((B+\tfrac{1}{4}+qE)^{1/2}+\tfrac{1}{2}+iA/2\sqrt{E}\right)+\tfrac{1}{2}\pi\left[\tfrac{1}{2}-(\tfrac{1}{4}+qE)^{1/2}\right]\ , \tag{22}$$

$$\frac{\partial}{\partial q}(\delta-\eta)=\frac{1}{2}E\left[\frac{\mathrm{Im}\psi_B}{(B+\frac{1}{4}+qE)^{1/2}}-\frac{\mathrm{Im}\psi_0}{(\frac{1}{4}+qE)^{1/2}}\right]+\frac{\pi E}{4}\left[\frac{1}{(\frac{1}{4}+qE)^{1/2}}-\frac{1}{(B+\frac{1}{4}+qE)^{1/2}}\right]\ , \tag{23}$$

where

$$\psi_B=\Psi\left((B+\tfrac{1}{4}+qE)^{1/2}+\tfrac{1}{2}+iA/2\sqrt{E}\right),\qquad \psi_0=\Psi\left((\tfrac{1}{4}+qE)^{1/2}+\tfrac{1}{2}+iA/2\sqrt{E}\right), \tag{24}$$

and $\Psi(z)$ is the digamma function. Thus we have

$$M(q_0)=\frac{2}{\pi\sqrt{E}}\int_{q_0}^{\infty}\left(\frac{\partial\delta}{\partial q}-\frac{\partial\eta}{\partial q}\right)\frac{dq}{(q-q_0)^{1/2}}=M_1(q_0)+M_2(q_0)\ , \tag{25}$$

where

$$M_1(q_0)=\frac{\sqrt{E}}{\pi}\int_{q_0}^{\infty}\left[\frac{\mathrm{Im}\psi_B}{(B+\frac{1}{4}+qE)^{1/2}}-\frac{\mathrm{Im}\psi_0}{(\frac{1}{4}+qE)^{1/2}}\right]\times\frac{dq}{(q-q_0)^{1/2}}\ , \tag{26}$$

$$M_2(q_0)=\frac{\sqrt{E}}{2}\int_{q_0}^{\infty}\left[\frac{1}{(\frac{1}{4}+qE)^{1/2}}-\frac{1}{(B+\frac{1}{4}+qE)^{1/2}}\right]\times\frac{dq}{(q-q_0)^{1/2}}\ . \tag{27}$$

$M_2(q_0)$ can be integrated and expressed in closed form as

$$M_2(q_0)=\tfrac{1}{2}\ln\left(1+\frac{B}{\frac{1}{4}+q_0E}\right)\ . \tag{28}$$

$M_1(q_0)$ has to be integrated numerically. We convert the infinite interval of integration into a finite one by the following change of variable:

$$q=\frac{q_0}{\sin^2\theta}\ ,$$

TABLE I. Construction of the potential (17) from phase shifts (19) and (20) at fixed energy $E=10$.

q_0	$r(q_0)$	$U_0(r(q_0))$	$U_0(r(q_0))+U_2(r(q_0))$	Real potential $U(r(q_0))$
0.2	0.590 85	4.3	4.8	4.6
0.5	0.823 35	2.6	2.70	2.69
0.7	0.944 01	2.15	2.189	2.181
1.0	1.098 90	1.72	1.740	1.738
2.0	1.499 59	1.106	1.111 8	1.111 5
5.0	2.308 76	0.619 8	0.620 76	0.620 74
7.0	2.714 98	0.503 5	0.503 997	0.503 990
10.0	3.228 40	0.405 5	0.405 698	0.405 696
20.0	4.533 57	0.269 17	0.269 231 3	0.269 231 0
50.0	7.128 31	0.159 956	0.159 965 84	0.159 965 82
70.0	8.422 72	0.132 817	0.132 822 454	0.132 822 446
100.0	10.055 12	0.109 340	0.109 342 460	0.109 342 457
200.0	14.195 76	0.075 405 3	0.075 405 873 5	0.075 405 873 2

TABLE II. Construction of the potential (17) from phase shifts (19) and (20) at fixed energy $E=100$.

q_0	$r(q_0)$	$U_0(r(q_0))$	$U_0(r(q_0))+U_2(r(q_0))$	Real potential $U(r(q_0))$
0.02	0.175 14	35.0	41.0	38.0
0.05	0.249 05	19.0	20.3	20.1
0.07	0.287 29	15.2	15.7	15.6
0.10	0.336 34	11.6	11.84	11.81
0.20	0.463 15	6.76	6.824	6.821
0.50	0.719 13	3.31	3.324 5	3.324 3
0.70	0.847 61	2.567	2.571 77	2.571 69
1.00	1.009 99	1.968	1.970 46	1.970 43
2.00	1.422 75	1.196 3	1.196 887	1.196 883
5.00	2.243 31	0.644 38	0.644 481 8	0.644 481 6
7.00	2.652 64	0.519 05	0.519 098 0	0.519 097 9
10.00	3.168 86	0.415 13	0.415 155 60	0.415 155 57
20.00	4.478 26	0.273 158	0.273 164 613	0.273 164 609
50.00	7.076 78	0.161 274	0.161 275 017 7	0.161 275 017 5
70.00	8.372 20	0.133 709 0	0.133 709 540 84	0.133 709 540 77
100.00	10.005 50	0.109 933 8	0.109 934 024 65	0.109 934 024 62
200.00	14.147 49	0.075 680 07	0.075 680 132 109	0.075 680 132 106

$$M_1(q_0)=\frac{4}{\pi}\left(\frac{q_0}{E}\right)^{1/2}\times\int_0^{\pi/2}\frac{d\theta}{\sin^2\theta}\left[\frac{\mathrm{Im}\psi_B}{(B+\frac{1}{4}+qE)^{1/2}}-\frac{\mathrm{Im}\psi_0}{(\frac{1}{4}+qE)^{1/2}}\right]_{q=q_0/\sin^2\theta}. \quad (29)$$

This integral is evaluated by the popular CADRE subroutine which can be readily called from IMSL. The error flag returned shows that it is well behaved.

After $M(q_0)$ has been determined, we can get $U_0(r(q_0))$ from

$$U(r(q_0))=E[1-q_0/r^2(q_0)] \quad (30)$$

and

$$r(q_0)=s(q_0)\exp(M(q_0)), \quad (31)$$

where

$$s(q_0)=[A+(A^2+4q_0E^2)^{1/2}]/2E. \quad (32)$$

To obtain the higher-order term, we need higher derivatives of s and r with respect to q_0E. They can be obtained by differentiating the logarithm of (31):

$$\ln r(q_0)=\ln s(q_0)+M_1(q_0)+M_2(q_0). \quad (33)$$

The digamma function is evaluated using the subroutine written by Kölbig.[5] The polygamma functions used in evaluating the higher derivatives are coded in the same way. We use the asymptotic expansions and recurrence formulas in Abramowitz and Stegun.[6]

We choose $A=B=1$ and vary q_0 at different energies. The results are given in Tables I and II. It is obvious that the constructed potential is less accurate as r approaches 0 because for $r<1$ the term B/r^2 dominates.

Since the generalized WKB approximation is essentially a semiclassical method, we expect more accurate results at higher energy. At $E=10$, the approximation breaks down at $r\simeq 0.5$. If we increase E to 100, this lower limit of r becomes 0.2. In the other extreme, as r approaches ∞, at $E=10$ and $r\simeq 14$, the constructed potential agrees with the real potential to 8 significant figures. At $E=100$ and $r\simeq 14$, the agreement is improved to 10 significant figures. In more realistic applications, there is an upper energy limit above which nonrelativistic scattering theory is no longer valid.

In conclusion, we have shown that the generalized WKB method is applicable to long-ranged potentials and the higher-order correction given by Vasilevsky *et al.* is extremely accurate.

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