PHYSICAL REVIEW A

GENERAL PHYSICS

THIRD SERIES, VOLUME 36, NUMBER 12 DECEMBER 15, 1987

Generalized WKB approximation to nonrelativistic normalizations and phase shifts in a screened Coulomb potential

J. Stein,* Akiva Ron,* I. B. Goldberg,* and R. H. Pratt
Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
(Received 17 April 1987)

We use the generalized WKB method with the Coulomb wave function as the comparison function to derive expressions for normalizations and phase shifts in a screened Coulomb potential as simple quadrature integrals. We compare our results with exact numerical results and with those of the standard WKB method. In most cases our results are good and more accurate than the standard WKB results. We also obtain the high-energy limits of our expressions and show that they coincide with the first-order high-energy-limit expansion of the analytic perturbation theory.

I. INTRODUCTION

The normalization of continuum wave functions and their phase shifts plays an important role in the calculation of various atomic processes, such as photoionization[1] and pair production.[2] We report here the results of applying a modified WKB method to the calculation of nonrelativistic normalizations and phase shifts in screened Coulomb potentials. As comparison functions we use nonrelativistic Coulomb wave functions; for a potential we consider the numerical self-consistent Herman-Skillman[3] potential with a long-range Latter tail.[4] We consider Coulomb functions corresponding to the nuclear charge, the ionic charge, and zero charge (the usual free function case). For each of these we consider both the original and the Langer-modified[5] forms. A preliminary report of some of our results has been given previously.[6] The idea of generalizing the exponential reference functions of the ordinary WKB method to solutions of an arbitrary Schrödinger equation was suggested by Miller and Good.[7] Subsequently Bartlett, Rice, and Good[8] applied this approach to the Schrödinger equation in the point Coulomb potential, utilizing free-particle spherical Bessel functions as comparison functions. The method was independently reinvented by Dingle,[9] who suggested a list of comparison functions. Recently, Durand and Durand[10] have discussed this approach, motivated by quark-confining potentials, considering as reference comparison functions spherical Bessel functions, Coulomb wave functions, and harmonic-oscillator wave functions.

Our own work is focused on the screened Coulomb potential appropriate for scattering in the field of an atom. We examine how well normalizations and phase shifts can be calculated with this approach, utilizing continuum Coulomb wave functions as our comparison functions. From this formalism we also obtain high-energy-limit expressions which can be compared with those which have been obtained in other ways.

It should be understood that we do not expect these WKB methods to be useful in actual calculations of wave-function *shapes*. The effort involved in solving the differential equation for the coordinate transformation function $\rho(R)$, together with the Coulomb functions, is not smaller than the effort involved in the direct numerical integration of the Schrödinger equation in a screened Coulomb potential. Rather, what we have achieved with this formalism are expressions for the normalizations and phase shifts, in terms of quadrature formulas. These expressions are simple to evaluate and relatively accurate.

In Sec. II we present the generalized WKB formalism, for clarity summarizing briefly some results from previous work[7,9] which we need for our derivation. In Sec. III we derive our results for the normalizations and phase shifts of continuum wave functions. In Sec. IV we derive the high-energy limits of our expressions and compare them with the analytic perturbation theory (APT).[11,12] In Sec. V we present our results and examine their accuracy, in comparison with direct numerical calculations. The study was carried out for carbon, aluminum, and iron, for energies in the range of 0.001–100 keV, and for angular momenta $l=0,1,2,4,10$. Results are generally very good, with the worst error in carbon for normalization being at the 10% level for $l=2$ at 10 eV, in phase shift at the 0.1-rad level for $l=1$ at 20 eV. These are situations in which the method could have been expected to become poor, in view of the proximity

to the double-well feature of the effective potential which has not been included in the derivation. Otherwise, one can obtain normalizations to at least 1% and phases to 0.01 rad (except for $l=0$).

II. GENERAL FORMALISM

We follow the nonrelativistic formulation of the generalized WKB method[7,8] to compute normalizations and phase shifts for continuum states in screened Coulomb potentials. We will concentrate on displaying normalizations and phase shifts rather than wave functions. Our aim is to find a WKB-type approximate solution to the radial Schrödinger equation

$$\frac{d^2Y(r)}{dr^2}+\left[\frac{2m}{\hbar^2}\left[E+\frac{Ze^2}{r}S(r)\right]-\frac{l(l+1)}{r^2}\right]Y(r)=0 , \tag{2.1}$$

where $S(r)$, the screening function, gives the modification of the Coulomb potential of point nuclear charge Z. Let us define (with η negative to conform with Ref. 13, Eq. 14.1.1)

$$p=\frac{\sqrt{2mE}}{\hbar},\quad \eta=-\frac{mZe^2}{\hbar^2 p}=-\frac{\alpha Z}{\lambda_c p} ,$$
$$\alpha=\frac{e^2}{\hbar c},\quad \lambda_c=\frac{\hbar}{mc} . \tag{2.2}$$

Then Eq. (2.1) becomes, for $\rho=pr$,

$$\frac{d^2Y(\rho)}{d\rho^2}+k_0^2(\rho)Y(\rho)=0 , \tag{2.3}$$

where

$$k_0^2(\rho)=1-\frac{2\eta s(\rho)}{\rho}-\frac{l(l+1)}{\rho^2} , \tag{2.4a}$$

and

$$s(\rho)=S\left[\frac{\rho}{p}\right]=S(r) \tag{2.4b}$$

is a function also of energy (p) for fixed ρ, although we have suppressed the energy dependence in our notation.

The generalized WKB method[7,9] assumes that we already know a solution of the equation

$$\frac{d^2U(R)}{dR^2}+K_0^2(R)U(R)=0 . \tag{2.5}$$

Here $U(R)$ is called the comparison function. We will look for an approximation $y(\rho)$ to $Y(\rho)$ which has the form

$$y(\rho)=A(\rho)U(R(\rho)) , \tag{2.6}$$

where $A(\rho)$ is a regular function to be determined. Inserting Eq. (2.6) into Eq. (2.3) and using Eq. (2.5) yields

$$U\left[\frac{d^2A}{d\rho^2}+k_0^2A-K_0^2A\left[\frac{dR}{d\rho}\right]^2\right]+\frac{dU}{dR}\left[2\frac{dA}{d\rho}\frac{dR}{d\rho}+A\frac{d^2R}{d\rho^2}\right]=0 . \tag{2.7}$$

Since $A(\rho)$ is arbitrary we can make the coefficient of dU/dR in Eq. (2.7) equal to zero by choosing

$$A^2(\rho)\frac{dR(\rho)}{d\rho}=C=\text{const} . \tag{2.8}$$

The physically interesting case is when $C\neq 0$. (If $C=0$, either $A=0$, in which case $y=0$, or $R=$const, in which case y is the same as A.) Now, the lowest-order WKB approximation is made in one of two ways: (i) by neglecting the second-order derivative $d^2A/d\rho^2$ (see Refs. 7 and 9) or (ii) by neglecting

$$\frac{d^2A}{d\rho^2}+\frac{A}{4}\left[\frac{1}{p^2}-\frac{1}{R^2}\left[\frac{dR}{d\rho}\right]^2\right]$$

(see Ref. 5). In either case we obtain, by (2.7) and (2.8),

$$\left[\frac{dR}{d\rho}\right]^2=\frac{k^2(\rho)}{K^2(R)} , \tag{2.9}$$

where

$$k^2(\rho)=1-\frac{2\eta s(\rho)}{\rho}-\frac{\Lambda^2}{\rho^2} ,$$
$$K^2(R)=1-\frac{2H}{R}-\frac{\Lambda^2}{R^2} , \tag{2.10}$$

while the expression for Λ depends on the choice noted above of the term to be neglected. In the first case above, $\Lambda=\sqrt{l(l+1)}$, and in the second case, $\Lambda=l+\frac{1}{2}$. Note, in the first case, $\Lambda=0$ for $l=0$, while in the second case, $\Lambda>0$ for all l; this is the origin of the improvement for s waves with Langer modification (second case). Given a solution for R; then A, which is assumed to be a regular function of ρ, is obtained from Eq. (2.8). For the sake of simplicity we impose two conditions on our comparison function and its argument: (a) We demand that $dR/d\rho$ should be nonsingular (hence A is nonzero). (b) The fundamental behavior of the comparison function near the origin ($R\rightarrow 0$) and in the asymptotic region ($R\rightarrow\infty$) should be similar to that of the exact wave function (when $\rho\rightarrow 0$ and ∞, respectively). If $\Lambda=0$ this will require preferably that $H=\eta$, certainly that $H\neq 0$. Therefore,

$$\frac{dR}{d\rho}=\frac{k(\rho)}{K(R)}>0 , \tag{2.11a}$$

which is equivalent to

$$\int^{\rho}k(x)dx=\int^{R}K(x)dx \tag{2.11b}$$

if the integrals exist. Thus a family of solutions R as a function of ρ is obtained. It also follows that if $k(\rho)$ is zero or singular at a point ρ_0 then $K(R(\rho))$ must also be zero or have singularity of the same order at $R_0=R(\rho_0)$

and vice versa. Equation (2.11b) then becomes

$$\int_{\rho_0}^{\rho} k(x)dx = \int_{R_0}^{R} K(x)dx \ . \tag{2.12}$$

This serves to define the desired particular solution in the family of solutions. Note that this can be satisfied by a single-valued real function $\rho(R)$ only if k and K have the same number of zeros and singularities. This can fail at low energies for effective atomic potentials of a given l with a double well, as in the barriers which lead to shape resonances. (The problem will also arise for bound states.) For l and energies near such a case the results will not be as good. Even if the problem arises for nonphysical l (i.e., noninteger), nearby physical l can be expected to be affected.

III. CONTINUUM WAVE FUNCTIONS

We now choose the comparison function $U(R)$ to be a regular solution of the Schrödinger equation in a point Coulomb potential of arbitrary nuclear charge and arbitrary positive energy but with the same angular momentum as in the original problem [cf. Eq. (2.1)]. We prefer the Coulomb function since it can have the same behavior near the origin or in the asymptotic region as the exact wave function.[10] We will discuss this point in Sec. IV. Thus we choose for Eq. (2.5)

$$K_0^2(R) = 1 - \frac{2H}{R} - \frac{l(l+1)}{R^2} \ . \tag{3.1}$$

Here H plays the role of η in Eq. (2.4). Since η combines nuclear charge and energy, choosing $H \neq \eta$ in our comparison function corresponds to changing nuclear charge or energy or both. $H=0$ corresponds to zero charge and the Bessel function as a comparison function. In the following, the actual choice of H in various situations will be made according to the nature of the particular problem we are going to solve.

We choose the normalizations of y and U such that the asymptotic behavior of the two functions is

$$y(\rho) = \sin\left[\rho - \bar{\eta}\ln 2\rho - l\frac{\pi}{2} + \sigma_{l,\bar{\eta}} + \delta\right] , \tag{3.2a}$$

$$U(R) = \sin\left[R - H\ln 2R - l\frac{\pi}{2} + \sigma_{l,H}\right] , \tag{3.2b}$$

where

$$\bar{\eta} = \lim_{\rho\to\infty} \eta s(\rho) = \eta s_\infty \ , \tag{3.3}$$

and the Coulomb phase is

$$\sigma_{l,\eta} = \arg\Gamma(l+1+i\eta) \ . \tag{3.4}$$

With this choice of the asymptotic behavior we have $A^2(\infty)=1$ and therefore $C=1$, and also

$$A^2(\rho) = \frac{1}{\frac{dR(\rho)}{d\rho}} = \frac{K(R)}{k(\rho)} \ . \tag{3.5}$$

A. Normalization

The normalization c_y of the continuum wave function $y(\rho)$ is defined here as $c_y = \lim_{\rho\to 0}[y(\rho)/\rho^{l+1}]$ when the asymptotic form of $y(\rho)$ is given by (3.2a). From Eqs. (2.6) and (3.5) we get

$$c_y = A(0)C_U \lim_{\rho\to 0}\left[\frac{R}{\rho}\right]^{l+1} = \frac{C_U}{A(0)^{2l+1}} \ , \tag{3.6}$$

where C_U is the coefficient of R^{l+1} in the expansion of the function $U(R)$ near the origin, which is given by Eq. (14.1.7) of Ref. (13) as

$$C_U = \frac{2^l e^{-(\pi/2)H}\,|\,\Gamma(l+1+iH)\,|}{(2l+1)!} \ . \tag{3.7}$$

One should remember that $A(0)$ also depends on l, or Eq. (3.6) will look even simpler than it is. In calculating $A(0)$ we distinguish between two cases according to the behavior of $k(\rho)$ and $K(R)$ near the origin.

1. $k(\rho)\sim\rho^{-1/2}$ $(\Lambda=0)$

In this case, assuming $H\neq 0$ (actually <0 corresponding to our choice $\eta<0$), there is one singular point, $\rho_0=0$ in $k(\rho)$ and $R_0=0$ in $K(R)$, so that Eq. (2.12) becomes

$$\int_0^{\rho} k(x)dx = \int_0^{R} K(x)dx \ . \tag{3.8}$$

Using Eq. (3.1) in the limit $\rho\to 0$ one gets

$$R = \frac{\eta}{H}\rho + O(\rho^2) \ , \tag{3.9}$$

so that by Eq. (3.5) we have

$$A(0) = \sqrt{H/\eta} \ . \tag{3.10}$$

It should be noted that for $l=0$ and $H=\eta$, as we have argued is preferred, the WKB normalization is equal to the Coulomb normalization. The near-independence of screening of s-wave normalizations (down to very low energy) has been observed in numerical calculations.

2. $k(\rho)\sim\rho^{-1}$ $(\Lambda>0)$

In this case $k(\rho)$ has a singular point $(\rho=0)$ and a zero at the classical turning point $\rho_0>0$. We notice that Eq. (3.8) cannot be used since the integrals diverge due to the centrifugal term. Defining

$$\begin{aligned} q^2(x) &= -k^2(x) \ , \\ Q^2(x) &= -K^2(x) \ , \end{aligned} \tag{3.11}$$

enables us to write Eq. (2.12) in the form

$$\int_{\rho}^{\rho_0}\left[q(x) - \frac{\Lambda}{x}\right]dx + \Lambda\ln\frac{\rho_0}{\rho} = \int_{R}^{R_0}\left[Q(x) - \frac{\Lambda}{x}\right]dx + \Lambda\ln\frac{R_0}{R} \ . \tag{3.12}$$

Equation (3.12) gives

$$\frac{\rho}{R}=\frac{\rho_0}{R_0}\exp\left\{\frac{1}{\Lambda}\left[\int_\rho^{\rho_0}\left[q(x)-\frac{\Lambda}{x}\right]dx - \int_R^{R_0}\left[Q(x)-\frac{\Lambda}{x}\right]dx\right]\right\}. \quad (3.13)$$

Using Eq. (3.5), we can write

$$A^2(0)=\left[\left.\frac{dR}{d\rho}\right|_{\rho=0}\right]^{-1}=\lim_{\rho\to 0}\frac{\rho}{R}$$
$$=\exp\left[\frac{1}{\Lambda}\lim_{\epsilon\to 0}\left[\int_\epsilon^{\rho_0}q(x)dx-\int_\epsilon^{R_0}Q(x)dx\right]\right]$$
$$=\exp\left[\frac{1}{\Lambda}\int_0^\infty \mathrm{Re}[q(x)-Q(x)]dx\right]. \quad (3.14)$$

Performing the integrals we get

$$A^2(0)=\rho_0\frac{R_0-H}{2\Lambda^2}\exp\left[\frac{1}{\Lambda}\int_0^{\rho_0}\left[q(x)-\frac{\Lambda}{x}\right]dx+1 - \frac{H}{\Lambda}\left[\frac{\pi}{2}+\arctan\frac{H}{\Lambda}\right]\right], \quad (3.15)$$

where

$$R_0=H+(H^2+\Lambda^2)^{1/2}$$

is a solution of the equation $K^2(R)=0$. If we set $H=\eta$ and $\Lambda=l+\frac{1}{2}$ in Eq. (3.15), we obtain Eq. (62) of Ref. 3, except for a missing factor of η in front of the $\tan^{-1}[\eta/(l+\frac{1}{2})]$ term in Eq. (62). Note that our η is negative, while η in Ref. 10 is positive.

B. Phase shifts

Here we are interested in the asymptotic behavior of the function $R(\rho)$ which satisfies Eq. (2.12). [Remember that $A^2(\infty)=1$.] For $\rho\to\infty$ we find [cf. Eqs. (2.4) and (3.3)]

$$k(\rho)=1-\frac{\bar\eta}{\rho}+O\left(\frac{1}{\rho^2}\right). \quad (3.16)$$

In order to avoid divergent integrals we rewrite the left-hand side of Eq. (2.12) in the following manner:

$$\int_{\rho_0}^{\rho}k(x)dx=\left[\int_{\rho_0}^{\rho}\left[k(x)-1+\frac{\bar\eta}{x}\right]dx-\rho_0+\bar\eta\ln 2\rho_0\right] +\rho-\bar\eta\ln 2\rho. \quad (3.17)$$

Denoting by f the limit of the expression in square brackets in Eq. (3.17) for $\rho\to\infty$, we have for very large values of ρ

$$\int_{\rho_0}^{\rho}k(x)dx\to f+\rho-\bar\eta\ln 2\rho. \quad (3.18)$$

Similarly, the right-hand side of Eq. (3.3) is

$$\int_{R_0}^{R}K(x)dx=\left[\int_{R_0}^{R}\left[K(x)-1+\frac{H}{x}\right]dx-R_0+H\ln 2R_0\right] +R-H\ln 2R,$$

which for $R\to\infty$ becomes

$$F+R-H\ln 2R. \quad (3.19)$$

(Note that both f and F converge in the limits $\rho_0\to 0$ and $R_0\to 0$ in the case $\Lambda=0$.) Equations (3.18) and (3.19) yield

$$R-H\ln 2R+F=\rho-\bar\eta\ln 2\rho+f+O(1). \quad (3.20)$$

Therefore,

$$R=\rho+(H-\bar\eta)\ln 2\rho+f-F+O(1). \quad (3.21)$$

Inserting these results into Eqs. (3.2a) and (3.2b) and equating the corresponding terms yields

$$\delta=f-F+\sigma_{l,H}-\sigma_{l,\bar\eta}. \quad (3.22)$$

Writing out the explicit expressions for f and F,

$$\delta=\sigma_{l,H}-\sigma_{l,\bar\eta}+H[1-\ln(R_0-H)]+\Lambda\left[\frac{\pi}{2}-\arctan\frac{H}{\Lambda}\right] +\int_{\rho_0}^{\infty}\left[k(x)-1+\frac{\bar\eta}{x}\right]dx-\rho_0+\bar\eta\ln 2\rho_0. \quad (3.23)$$

We can get a more symmetric expression if instead of subtracting $1-\bar\eta/x$ from $k(x)$ we subtract

$$\bar k(x)=\left[1-\frac{2\bar\eta}{x}-\frac{\lambda^2}{x^2}\right]^{1/2}, \quad (3.24)$$

which has the same asymptotic form as $x\to\infty$. Noting that $\mathrm{Re}[k(x)]=k(x)$ when $x>\rho_0$ and vanishes when $x\le\rho_0$, we get

$$\delta=\sigma_{l,H}+H[1-\ln(H^2+\Lambda^2)^{1/2}]-\Lambda\arctan\frac{H}{\Lambda} -\left[\sigma_{l,\bar\eta}+\bar\eta[1-\ln(\bar\eta^2+\Lambda^2)^{1/2}]-\Lambda\arctan\frac{\bar\eta}{\Lambda}\right] +\int_0^\infty \mathrm{Re}[k(x)-\bar k(x)]dx. \quad (3.25)$$

IV. HIGH-ENERGY LIMIT ($p\to inf$, $\eta\to 0$)

A. Normalization

For $\Lambda=0$ we have $A^2(0)=H/\eta$ [Eq. (3.10)]. For $\Lambda>0$ we assume that in the high-energy limit H also tends to zero. Then, from Eqs. (3.14) and (2.4) we get

$$A^2(0)\approx 1+\frac{\pi}{2}\frac{\eta-H}{\Lambda}+\frac{1}{2}\left[\frac{\pi}{2}\frac{\eta-H}{\Lambda}\right]^2+\frac{3}{2}\frac{\eta^2-H^2}{\Lambda^2} -\eta^2\frac{\lambda_0}{\alpha Z}\frac{dS(0)}{dr}. \quad (4.1)$$

The normalization C_y is given by Eq. (3.6). On substituting $H=\eta$ we get

$$\frac{C_y}{C_U}=1, \quad \Lambda=0 ,$$
$$\frac{C_y}{C_U}=A(0)^{-(2l+1)}\approx 1+(l+\tfrac{1}{2})\frac{\lambda_c}{\alpha Z}\frac{dS(0)}{dr}\eta^2, \quad \Lambda>0 . \tag{4.2}$$

B. Phase shifts

Defining

$$I(\rho_1)=\int_{\rho_0}^{\rho_1} k(x)dx , \tag{4.3}$$

the integral in Eq. (3.23) is

$$\int_{\rho_0}^{\infty}\left[k(x)-1+\frac{\bar{\eta}}{x}\right]dx = \lim_{\rho_1\to\infty}\left[I(\rho_1)-(\rho_1-\rho_0)+\bar{\eta}\ln\frac{\rho_1}{\rho_0}\right] . \tag{4.4}$$

For small enough $|\eta|$ we can find a constant ρ_m such that the following two conditions hold:

$$1-s(x)=1-S\left[-\frac{\lambda_c\eta}{\alpha Z}x\right]\ll 1 \quad \text{for } \rho_0\le x\le\rho_m , \tag{4.5a}$$
$$|2\eta x| \ll x^2-\Lambda^2 \quad \text{for } \rho_m\le x . \tag{4.5b}$$

We divide $I(\rho_0)$ into two integrals:

$$I(\rho_1)=\int_{\rho_0}^{\rho_m}k(x)dx+\int_{\rho_m}^{\rho_1}k(x)dx=I_1+I_2 . \tag{4.6}$$

Defining

$$t(x)=(x^2-\Lambda^2)^{1/2} , \tag{4.7}$$

then to first order in η we get

$$I_1=\int_{\rho_0}^{\rho_m}(x^2-2x\eta-\Lambda^2)^{1/2}dx \approx t(\rho_m)+\Lambda\left[\tan^{-1}\frac{\Lambda}{t(\rho_m)}-\frac{\pi}{2}\right]-\eta\ln[\rho_m+t(\rho_m)] +\frac{\eta}{2}\ln(\Lambda^2+\eta^2) , \tag{4.8}$$

$$I_2=\int_{\rho_m}^{\rho_1}t(x)\left[1-\frac{\eta x s(x)}{t^2(x)}\right]\frac{dx}{x} \approx t(\rho_1)+\Lambda\tan^{-1}\frac{\Lambda}{t(\rho_1)}-t(\rho_m)-\Lambda\tan^{-1}\frac{\Lambda}{t(\rho_m)} -\eta\{s_\infty\ln[\rho_1+t(\rho_1)]-\ln[\rho_m+t(\rho_m)]\} +\eta\int_{\rho_m/\rho}^{\rho_1/\rho}\frac{dS(r)}{dr}\ln[pr+t(pr)]dr . \tag{4.9}$$

Inserting I_1 and I_2 in Eq. (4.4), going to the limit $\rho_1\to\infty$, and inserting the results in Eq. (3.23), we get

$$\delta\approx\sigma_{l,H}-\sigma_{l,\bar{\eta}}+\frac{\eta}{2}\ln(\Lambda^2+\eta^2)-\frac{H}{2}\ln(\Lambda^2+H^2) +\eta\int_0^\infty\frac{dS(r)}{dr}\ln 2pr\,dr . \tag{4.10}$$

When $\Lambda\neq 0$ we can ignore η^2 and H^2 in the logarithmic terms. Setting $H=\eta$ and $\bar{\eta}=0$, Eq. (4.10) agrees with the first-order term in the $1/p$ expansion of the phase shifts given by Bechler and Pratt.[12]

V. RESULTS AND DISCUSSION

We present in Tables I and II some numerical results which illustrate the utility of our generalized WKB expressions. We consider the Herman-Skillman[3] self-consistent field (with Latter tail) for carbon. We consider the three choices $H=0,\bar{\eta},\eta$ combined with the two choices $\Lambda_1=[l(l+1)]^{1/2}$, $\Lambda_2=l+\frac{1}{2}$. For each of these six cases we show the predictions for normalizations and phase shifts, for $l=0,2,10$ and energies from 1 eV to 100 keV (by decade). The integrals appearing in the approximate expressions for the normalization [Eq. (3.15)] and for the phase shift [Eq. (3.25)] were computed numerically, using values of the screening function obtained by interpolation of a numerically generated potential table. In Table I we show the "exact" numerical results for the ratio of normalization in the potential to the nuclear point Coulomb normalization, together with the relative error of the various WKB forms. In Table II we show the "exact" numerical results for phase shifts δ, i.e., the difference of phase from the Latter-tail Coulombic $\sigma_{l,\bar{\eta}}$ together with the absolute error of our various WKB forms. We note that for $\Lambda_1=0$, for which $H=0$ is unacceptable, results for $H=\bar{\eta}$ are much poorer than for $H=\eta$ (except for very low energy), as we had predicted. At high energy the normalization approaches the nuclear point Coulomb value (more slowly for high l); the phase shift vanishes and phase-shift *differences* approach nuclear point Coulomb values, as is predicted by Eq. (4.10). At low energy the phase shift (relative to the Latter-tail Coulombic phase shift) vanishes if there are no bound states of the given angular momentum (generalized Levinson's theorem). For normalizations, Table I indicates that Λ_2 is always the best choice, more so at high energy (and especially for $l=0$). $H=\eta$ is better for low l and high energy; $H=\bar{\eta}$ is better for high l and low energy. $H=0$ is poor for low l and low energy; otherwise, it is adequate though not generally optimum. For phase shifts, Table II indicates that Λ_2 is again better than Λ_1, while η is now better than $\bar{\eta}$ in all cases. In general, we obtain an accuracy of at least 1% for normalizations, 0.01 rad for phases. Results are worse for $l=1$ and $l=2$ at 10–20 eV. This is connected with the fact that the effective potential for carbon develops a double well for unphysical l (1.4–1.6) between these values. As originally indicated, for such l and for energies comparable with such structures, our procedures would not be expected to work as well.

TABLE I. Relative error of the generalized WKB approximation for the normalization of carbon continuum wave functions of various angular momentum l and energy E, using the choices $H=0$, $\bar{\eta}$ or η, and $\Lambda^2=l(l+1)$ or $(l+\frac{1}{2})^2$. Also shown is the ratio of exact screened to nuclear point Coulomb normalization in the same Herman-Skillman potential. Here $a\times 10^m$.

			Relative error of WKB (Λ^2,H)					
		Exact	$\Lambda^2=l(l+1)$			$\Lambda^2=(l+\frac{1}{2})^2$		
l	E (keV)	ratio	$H=0$	$\bar{\eta}$	η	$H=0$	$\bar{\eta}$	η
0	0.001	9.52[−1]		5.1[−2]	5.1[−2]	−3.2[−2]	3.9[−2]	4.1[−2]
0	0.010	9.67[−1]		3.4[−2]	3.4[−2]	−4.7[−2]	1.0[−2]	2.4[−2]
0	0.100	9.99[−1]		5.4[−2]	8.9[−4]	−7.4[−2]	−5.6[−2]	8.2[−3]
0	1.000	9.99[−1]		3.8[−1]	9.1[−4]	−4.6[−2]	−4.4[−2]	6.3[−3]
0	10.000	9.98[−1]		9.1[−1]	2.3[−3]	−8.1[−3]	−7.9[−3]	2.9[−4]
0	100.000	10.00[−1]		1.2[+0]	4.0[−4]	−8.7[−4]	−8.4[−4]	8.0[−6]
2	0.001	5.83[−2]	1.2[−1]	8.1[−2]	8.1[−2]	−1.8[−2]	−7.1[−3]	2.1[−3]
2	0.010	1.33[−1]	2.3[−1]	2.0[−1]	1.9[−1]	9.5[−2]	9.8[−2]	1.1[−1]
2	0.100	4.37[−1]	5.5[−2]	4.4[−2]	2.3[−2]	3.9[−3]	4.2[−3]	1.1[−2]
2	1.000	8.32[−1]	2.0[−2]	1.6[−2]	2.0[−3]	−6.7[−5]	−5.5[−5]	1.1[−3]
2	10.000	9.75[−1]	6.8[−3]	5.6[−3]	1.7[−4]	−2.9[−5]	−2.9[−5]	8.4[−5]
2	100.000	9.97[−1]	2.2[−3]	1.8[−3]	8.0[−6]	−1.2[−5]	−1.2[−5]	2.0[−6]
10	0.001	1.74[−6]	5.5[−3]	6.9[−4]	−3.2[−3]	−4.6[−4]	5.7[−5]	2.9[−3]
10	0.010	1.16[−3]	2.6[−3]	7.0[−4]	−4.1[−3]	−7.8[−5]	8.6[−6]	1.1[−3]
10	0.100	9.22[−2]	1.2[−3]	5.9[−4]	−2.0[−3]	−9.5[−5]	−8.5[−5]	1.0[−4]
10	1.000	5.61[−1]	1.0[−3]	8.2[−4]	−1.6[−4]	1.8[−4]	1.8[−4]	1.8[−4]
10	10.000	9.07[−1]	4.0[−4]	3.3[−4]	1.3[−5]	3.5[−5]	3.5[−5]	3.5[−5]
10	100.000	9.88[−1]	1.2[−4]	1.02[−4]	1.0[−6]	1.0[−6]	1.0[−6]	1.0[−6]

TABLE II. Error of the generalized WKB approximation for the phase shifts δ of carbon continuum wave functions of various angular momenta l and energy E, using the choices $H=0$, $\bar{\eta}$ or η, and $\Lambda^2=l(l+1)$ or $(l+\frac{1}{2})^2$. Also shown is the difference between exact screened and nuclear point Coulomb phase shifts in the same Herman-Skillman potential. Note that the full phase shift is $\delta+\sigma_{l,\bar{\eta}}$, where $\sigma_{l,\bar{\eta}}$ is the phase shift in the Latter-tail Coulomb potential.

			Error of WKB (Λ^2,H)					
		Exact	$\Lambda^2=l(l+1)$			$\Lambda^2=(l+\frac{1}{2})^2$		
l	E (keV)	difference	$H=0$	$\bar{\eta}$	η	$H=0$	$\bar{\eta}$	η
0	0.001	3.06		0.08	0.06	−0.03	−0.07	−0.06
0	0.010	2.92		0.13	0.06	−0.05	−0.05	−0.03
0	0.100	2.35		0.24	0.04	−0.07	−0.02	−0.01
0	1.000	1.37		0.37	0.02	−0.05	0.03	0.00
0	10.000	0.64		0.30	0.00	−0.01	0.02	0.00
0	100.000	0.27		0.16	−0.00	−0.00	0.01	−0.00
2	0.001	0.04	0.02	−0.04	−0.05	−0.02	−0.04	−0.03
2	0.010	0.14	0.07	0.05	0.01	0.09	0.00	0.01
2	0.100	0.58	0.04	0.03	−0.00	0.00	0.01	0.00
2	1.000	0.57	0.02	0.01	−0.00	−0.00	0.00	0.00
2	10.000	0.36	0.01	0.01	−0.00	−0.00	0.00	0.00
2	100.000	0.18	0.00	0.00	−0.00	−0.00	0.00	−0.00
10	0.001	0.00	0.01	−0.00	−0.01	−0.00	−0.00	−0.00
10	0.010	0.00	0.00	0.00	−0.01	−0.00	0.00	−0.00
10	0.100	0.00	0.00	0.00	−0.00	−0.00	0.00	−0.00
10	1.000	0.07	0.00	0.00	−0.00	0.00	0.00	−0.00
10	10.000	0.13	0.00	0.00	−0.00	0.00	0.00	−0.00
10	100.000	0.10	0.00	0.00	−0.00	0.00	−0.00	−0.00

The high-energy expression, Eq. (4.2), for the normalization, which becomes increasingly accurate with increasing energy, gives very good results for the case $l=0$, in which screening effects remain small down to a few eV. The relative error with respect to the exact result amounts to ≈ 0.003 for $E=10$ keV and to ≈ 0.001 at 100 keV. The relative error increases with l; it is ≈ 0.015 at 10 keV and ≈ 0.0011 at 100 keV for $l=10$. The high-energy expression, Eq. (4.10), for the phase shift gives good results for energies above 5 keV, where the difference from the exact value amounts to less than 0.005 rad for small l values. The results are not as good for $l=10$, where the difference is only $\lesssim 0.08$ rad.

ACKNOWLEDGMENTS

We thank Professor R. H. Good, Jr. for encouragement and helpful remarks. We are also indebted to Dr. B. J. B. Crowley for bibliographic help.

---

*Permanent address: Racah Institute of Physics, Hebrew University of Jerusalem, Jerusalem 91905, Israel.

[1]A. Bechler, R. Dutt, S. K. Sen Gupta, and R. H. Pratt, Nucl. Instrum. Methods A **255**, 43 (1987), with details in A. Bechler, University of Pittsburgh, Internal Report No. PITT-347 (unpublished).

[2]H. K. Tseng and R. H. Pratt, Phys. Rev. A **6**, 2049 (1972); **21**, 454 (1980).

[3]F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, NJ, 1963).

[4]R. Latter, Phys. Rev. **99**, 510 (1955).

[5]R. E. Langer, Phys. Rev. **51**, 669 (1937).

[6]A. Ron, I. B. Goldberg, J. Stein, and R. H. Pratt, Bull. Isr. Phys. Soc., 79 (1985).

[7]S. C. Miller, Jr. and R. H. Good, Jr., Phys. Rev. **91**, 174 (1953).

[8]R. H. Bartlett, M. H. Rice, and R. H. Good, Jr., Ann. Phys. **2**, 372 (1957).

[9]R. B. Dingle, Appl. Sci. Res. B **5**, 345 (1956).

[10]B. Durand and L. Durand, Phys. Rev. A **33**, 2887 (1986).

[11]J. McEnnan, L. Kissel, and R. H. Pratt, Phys. Rev. A **13**, 532 (1976).

[12]A. Bechler and R. H. Pratt, Phys. Rev. A **28**, 1190 (1983); Ann. Phys. **163**, 28 (1985).

[13]*Handbook of Mathematical Functions,* Natl. Bur. Stand. Appl. Math. Ser. No. 55, edited by M. Abramowitz and I. Stegun (U.S. GPO, Washington, D.C., 1965).