PHYSICAL REVIEW VOLUME 106, NUMBER 6 JUNE 15, 1957

Extension of the WKB Equation

CHARLES E. HECHT*† AND JOSEPH E. MAYER
Enrico Fermi Institute for Nuclear Studies, University of Chicago, Chicago, Illinois
(Received March 15, 1957)

The WKB form suitable for the classical region of potential energy less than the total energy, $\psi(x)=(dz/dx)^{-\frac{1}{2}}\sin z$, is used to obtain a function $z(x)$ that reproduces the time-independent Schrödinger equation solutions $\psi(x)$, to any desired degree of accuracy through the turning point and into the nonclassical region.

1. INTRODUCTION

THE Wentzel-Kramers-Brillouin method has been useful for the approximation of the solution to the time-independent Schrödinger equation. The normal approximative method uses two forms, one applicable to the "classical" region for which the energy is greater than the potential, and the other applicable to the "nonclassical" region for which the potential exceeds the total energy. The function is not represented through the "turning point" for which the total energy and the potential energy become equal. We propose a simple form for the argument, $z(x)$, of the "classical" approximation, which form makes this single solution valid in both regions. This *zero*th approximation can, in turn, be improved to any desired accuracy.

2. THE PROBLEM

The one-dimensional time-independent Schrödinger equation can be written

$$d^2\psi(x)/dx^2+\gamma(x)\psi(x)=0, \tag{1}$$

with

$$\gamma(x)=\epsilon_n-u(x), \tag{2}$$

and

$$\epsilon_n=(2m/\hbar^2)E_n, \tag{3a}$$

$$u(x)=(2m/\hbar^2)U(x), \tag{3b}$$

in which E_n is the energy of the nth level and $U(x)$ the potential energy in conventional units. The quantity γ has dimensions L^{-2}.

Equation (1) is a linear differential equation of second order, the solutions of which can be mapped onto the solutions of any other convenient linear differential equation of second order by use of the Schwarzian derivative formalism.[1–4] Using this, we may say that $\phi(z)$ is a solution of

$$d^2\phi/dz^2+R(z)\phi(z)=0, \tag{4}$$

with $R(z)$ any arbitrary function of z, and z itself considered as a function of x. We then have

$$\psi(x)=z_1^{-\frac{1}{2}}\phi[z(x)], \tag{5}$$

in which

$$z_1=dz/dx,\quad z_2=d^2z/dx^2,\quad \text{etc.}, \tag{6}$$

provided z obeys the equation,

$$R(z)=z_1^{-2}[\gamma-\tfrac{1}{2}\langle z;x\rangle], \tag{7}$$

where $\langle z;x\rangle$ is the Schwarzian derivative:

$$\langle z;x\rangle=-2z_1^{\frac{1}{2}}\frac{d^2}{dx^2}(z_1^{-\frac{1}{2}})=\frac{z_3}{z_1}-\frac{3}{2}\left(\frac{z_2}{z_1}\right)^2. \tag{8}$$

All this can be readily checked by using (5) in (1), with (7) for z_1, after eliminating $d^2\phi/dz^2$ with the aid of (4).

The usual use of this mapping is to choose $R(z)$ to be some simple analytic expression for which ϕ is known, but for which R and γ resemble each other. In this case $\langle z;x\rangle$ can be neglected, at least in a crude approximation, since then the solution,

$$R^{\frac{1}{2}}z_1=\gamma^{\frac{1}{2}}, \tag{9}$$

leads to z_1 approximately equal to a constant, $\langle z;x\rangle\approx 0$. If $\gamma(x)$ is large and positive, and does not vary rapidly with x, one may choose $R\equiv 1$, $\phi(z)=\sin z$ or $\cos z$, namely,

$$\psi(x)=z_1^{-\frac{1}{2}}\sin z(x). \tag{10}$$

This will be an exact relationship if $z(x)$ is the solution of the equation

$$z_1^2+\tfrac{1}{2}\langle z;x\rangle=\gamma(x). \tag{11}$$

* Present address: Naval Research Laboratory, Department of Chemistry, University of Wisconsin, Madison, Wisconsin.

† Part of a dissertation submitted in partial fulfillment of the requirements for the Ph.D., Department of Chemistry, University of Chicago.

[1] A. R. Forsyth, *A Treatise on Differential Equations* (The Macmillan Company, New York, 1929), sixth edition, pp. 104, 230.

[2] Per O. Löwdin has called our attention to the convenience of this method and to his unpublished notes thereon in the Quarterly Progress Report of the Massachusetts Institute of Technology Solid State and Molecular Theory Group, January, 1952.

[3] Since the development of this paper we have noted the work of R. B. Dingle, Appl. Sci. Research **B5**, 345 (1956), which discusses several mappings for solving linear second-order differential equations. However, we believe that the iteration scheme to be evolved in this paper is sufficiently felicitous to merit separate publication.

[4] S. C. Miller and R. H. Good, Phys. Rev. **91**, 174 (1953). These authors have also written of mappings and the WKB method but again not in such a way as to obtain a general iteration scheme.

The approximate solution, $z^{(0)}(x)$, given by

$$z^{(0)}(x)=\int^x [\gamma(x)]^{\frac{1}{2}}dx, \tag{12a}$$

$$\psi(x)\approx[z_1^{(0)}(x)]^{-\frac{1}{2}}\sin z^{(0)}(x) \tag{12b}$$

is then the conventional WKB[5] approximation for the classical region in which $\gamma(x)\gg 0$, $\epsilon_n \ll u(x)$.

An alternative for $\gamma(x)\ll 0$, is to choose a different mapping variable, y, $R(y)=-1$, $\phi(y)=e^{-y}$, so that the zeroth approximation is

$$y^{(0)}(x)=\int^x [-\gamma(x)]^{\frac{1}{2}}dx, \tag{13a}$$

$$\psi(x)\approx[y_1^{(0)}]^{-\frac{1}{2}}\exp[-y^{(0)}(x)]. \tag{13b}$$

We emphasize here that the y and z are utterly different functions of x. These, then, are the two simple WKB approximations for $\psi(x)$ in the classical and nonclassical regions respectively, both of which become singular at the turning point, $\gamma(x)=0$.

It is quite possible, by choosing R other than a constant, to find functions ϕ on which the mapping through the turning point offers no difficulties. If $R(z)$ is linear, the mapping is on the Airy integrals,[3,6] whereas a quadratic $R(z)$ enables one to map on the Hermite functions[4] through two turning points. There is, however, a certain simplicity in the mapping on a sine or cosine function, $R\equiv 1$, since in this case, $z(x)$ approaches the classical action variable in the limit $\epsilon_n \gg u(x)$. We propose to show a method by which the $z(x)$ defined by Eq. (11) can be obtained with arbitrary accuracy through the turning point for which $\gamma=0$, which point is *not* a singular point of the differential equation (11).

The essence of the method is to produce a real positive function, $z^{(0)}(x)$, which is a satisfactory zeroth approximation to $z(x)$ in both the classical and nonclassical region, such that $(dz^{(0)}/dx)^{-\frac{1}{2}}\sin z^{(0)}$ becomes asymptotically equal to the classical and nonclassical WKB approximations in the regions of large magnitude of γ, positive and negative respectively, and for which $(dz^{(0)}/dx)^{-\frac{1}{2}}\sin z^{(0)}$ remains regular through $\gamma=0$. We then show that the solution, $z(x)$, of (11) can be computed from this $z^{(0)}(x)$ with any desired accuracy. The method does, however, require that the dependence of $\gamma(x)$ on x should not be excessively pathological in nature, namely that successive derivatives $d^\nu\gamma/dx^\nu$ decrease appropriately for large ν values, and that $d\gamma/dx\equiv\gamma_1$ be non-zero at the turning point.

3. FORMAL GENERAL SOLUTION

To specify the problem more closely consider the case that the zero of x is chosen to be at the turning point, and that γ_1 is positive. We have

$x<0$, $\gamma<0$, nonclassical;
$x=0$, $\gamma=0$, turning point;
$x>0$, $\gamma>0$, classical.

We may write Eq. (11) as

$$z_1^2-z_1^{\frac{1}{2}}\frac{d^2}{dx^2}(z_1^{-\frac{1}{2}})=\gamma(x), \tag{14}$$

and our eigenfunction as

$$\psi=z_1^{-\frac{1}{2}}\sin z=z_1^{-\frac{1}{2}}\sin\int_{-\infty}^x z_1 dx, \tag{15}$$

in which we have imposed the condition $\psi(-\infty)=0$.

To develop a form for z_1 amenable to iteration, we make use of two nice properties of Schwarzian derivatives. As we have seen, if $\psi(x)$ obeys the equation $d^2\psi/dx^2+\gamma\psi=0$, and $\phi(z)$ the relation $d^2\phi/dz^2+R\phi=0$, then $\psi=(dz/dx)^{-\frac{1}{2}}\phi$ if (7) obtains. Similarly, $\phi=(dx/dz)^{-\frac{1}{2}}\psi$ if

$$\gamma(x)=(dx/dz)^{-2}[R-\tfrac{1}{2}\langle x;z\rangle]. \tag{16}$$

Compare this with (7) to derive

$$\langle z;x\rangle=-(dz/dx)^2\langle x;z\rangle. \tag{17}$$

Now suppose $\theta(\eta)$ obeys the relation $d^2\theta/d\eta^2+Q\theta=0$. One can obtain equations from equating $\psi=(d\eta/dx)^{-\frac{1}{2}}\theta$ or $\phi=(d\eta/dx)^{-\frac{1}{2}}\theta$. With (7) these are

$$(dz/dx)^2+\tfrac{1}{2}\langle z;x\rangle=\gamma(x), \tag{18a}$$

$$Q(d\eta/dx)^2+\tfrac{1}{2}\langle \eta;x\rangle=\gamma(x), \tag{18b}$$

$$(dz/d\eta)^2+\tfrac{1}{2}\langle z;\eta\rangle=Q(\eta). \tag{18c}$$

Use γ in (18a) from (18b) replacing Q by (18c). One finds

$$\langle z;x\rangle=\langle \eta;x\rangle+(d\eta/dx)^2\langle z;\eta\rangle. \tag{19}$$

Multiplication of (18a) by $(dx/d\eta)^2$ and substitution of (19) for $\langle z;x\rangle$ in the resulting form yields a relation which holds for *any* function η:

$$(dz/d\eta)^2+\tfrac{1}{2}\langle z;\eta\rangle=(d\eta/dx)^{-2}[\gamma-\tfrac{1}{2}\langle\eta;x\rangle]. \tag{20}$$

This equation now serves as a possible iteration equation. If η is such that the right hand side of (20) is exactly unity, then η_1 is exactly the correct solution, $\eta_1\equiv z_1$ of Eq. (11), and (20) gives $dz/d\eta=1$. If, however, η is an approximate solution, say $\eta=z^{(\nu)}$, so that the right hand side of (20) is nearly unity, then the approximation of neglecting $\langle z;\eta\rangle$ on the left leads to a better solution $z^{(\nu+1)}$ as

$$dz^{(\nu+1)}/dz^{(\nu)}=(dz^{(\nu)}/dx)^{-1}[\gamma-\tfrac{1}{2}\langle z^{(\nu)};x\rangle]^{\frac{1}{2}}. \tag{20'}$$

Actually, however, in order to use this scheme we must choose $z^{(\nu)}$ such that the quantity under the radical always remains positive.

[5] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), first edition, p. 178.
[6] J. C. P. Miller, *The Airy Integral*, British Association Mathematical Tables (Cambridge University Press, Cambridge, 1946).

We prefer, however, an alternative iteration method which has the advantage of leading us directly to an acceptable equation for $z^{(0)}$, namely one in which the Schwarzian $\frac{1}{2}\langle z;\eta\rangle$ on the left of (20) is replaced by $\frac{1}{2}\langle \ln z;\ln\eta\rangle$, so that instead of neglecting $\langle z;\eta\rangle$ in successive iterations the neglect is of $\langle \ln z;\ln\eta\rangle$. To carry this out, write

$$\begin{aligned} z&=e^{\lambda}, & \lambda&=\ln z, \\ z^{(\nu)}&=e^{\eta}, & \eta&=\ln z^{(\nu)}. \end{aligned} \tag{21}$$

We then express $\langle\eta;x\rangle$ in terms of derivatives of $z^{(\nu)}$ as

$$\tfrac{1}{2}\langle\eta;x\rangle=\tfrac{1}{4}[z_1^{(\nu)}/z^{(\nu)}]^2+\tfrac{1}{2}\langle z^{(\nu)};x\rangle \tag{22}$$

from (8), and $\langle z;\eta\rangle$ in terms of $\langle\lambda;\eta\rangle$ as

$$\tfrac{1}{2}\langle\lambda;\eta\rangle=\frac{1}{4z^2}\left(\frac{dz}{d\eta}\right)^2+\tfrac{1}{2}\langle z;\eta\rangle \tag{22$'$}$$

to find that, after multiplication of (20) by $(d\eta/dx)^2$ [noting that $(dz/d\eta)(d\eta/dx)=dz/dx=z_1$],

$$\left(1-\frac{1}{4z^2}\right)z_1^2+\frac{1}{2}\left(\frac{d\eta}{dx}\right)^2\langle\lambda;\eta\rangle=\gamma-\tfrac{1}{2}\langle z^{(\nu)};x\rangle-\frac{1}{4}\left(\frac{z_1^{(\nu)}}{z^{(\nu)}}\right)^2.$$

Elimination of λ and η from the notation by use of (21) leads to

$$\left(1-\frac{1}{4z^2}\right)z_1^2+\frac{1}{2}\left(\frac{z_1^{(\nu)}}{z^{(\nu)}}\right)^2\langle\ln z;\ln z^{(\nu)}\rangle =\gamma-\tfrac{1}{2}\langle z^{(\nu)};x\rangle-\frac{1}{4}\left(\frac{z_1^{(\nu)}}{z^{(\nu)}}\right)^2. \tag{23}$$

We may check (23) by noting that if $z^{(\nu)}$ is the correct solution $z^{(\nu)}\equiv z$, so that the Schwarzian derivative $\langle\ln z;\ln z^{(\nu)}\rangle$ is zero, the equation is just Eq. (8) with the added term $-\frac{1}{4}(z_1/z)^2=-\frac{1}{4}(z_1^{(\nu)}/z^{(\nu)})^2$ on each side.

Equation (23) is now exact, with $z^{(\nu)}$ any approximate solution. We write the $(\nu+1)$th approximation by omitting the term $\langle\ln z;\ln z^{(\nu)}\rangle$ on the left, as

$$\begin{aligned} z_1^{(\nu+1)}&=dz^{(\nu+1)}/dx \\ &=[\gamma+q(z^{(\nu)})]^{\frac{1}{2}}[1-(2z^{(\nu+1)})^{-2}]^{-\frac{1}{2}}, \end{aligned} \tag{24}$$

with

$$\begin{aligned} q(z)&=-(z_1/2z)^2-\frac{1}{2}\frac{z_3}{z_1}+\frac{3}{4}\left(\frac{z_2}{z_1}\right)^2 \\ &=-\left(\frac{1}{2}\frac{d}{dx}\ln z\right)^2-\left(\frac{1}{2}\frac{d^2}{dx^2}\ln\frac{dz}{dx}\right) \\ &\quad+\left(\frac{1}{2}\frac{d}{dx}\ln\frac{dz}{dx}\right)^2. \end{aligned} \tag{25}$$

4. ZEROTH-ORDER SOLUTION

We call the zeroth-order solution that obtained from (24) by setting $z^{(\nu)}$ equal to a constant, so that $q(z)=0$, or, omitting the superscript zero which indicates the order, we use the equation,

$$dz/dx=\left[\frac{\gamma}{1-(1/4z^2)}\right]^{\frac{1}{2}}, \tag{26}$$

with the boundary condition at the turning point,

$$z(x=0)=\tfrac{1}{2},\quad \gamma(x=0)=0. \tag{27}$$

The asymptotic solutions of (26), that is,

$$z(x)\cong c+\int_0^x[\gamma(y)]^{\frac{1}{2}}dy,\qquad x\gg0,\ \gamma\gg0 \tag{28a}$$

$$z(x)\cong\tfrac{1}{2}\exp\left[-2\int_x^0[-\gamma(y)]^{\frac{1}{2}}dy\right],\qquad x\ll0,\ \gamma\ll0 \tag{28b}$$

lead to the known WKB solutions,

$$\psi(x)=(dz/dx)^{\frac{1}{2}}\sin z \tag{29}$$

$$\cong\gamma^{-\frac{1}{4}}\sin\left[\int_0^x\gamma^{\frac{1}{2}}dy\right],\qquad x\gg0 \tag{29a}$$

$$\cong(-\gamma)^{-\frac{1}{4}}\exp\left[-\int_x^0(-\gamma)^{\frac{1}{2}}dy\right],\qquad x\ll0 \tag{29b}$$

for the classical and nonclassical regions, respectively. The latter form, (29b), is obtained by setting $\sin z\cong z$, $z\ll1$. The function z of (26) is regular through the turning point.

We may proceed to obtain expressions for the function $z(x)$ in the three regions, $x\gg0$, $x\cong0$, $x\ll0$, in terms of the two dimensionless *positive* integrals,

$$\beta_c(x)=\int_0^x[\gamma(y)]^{\frac{1}{2}}dy=\int_0^x\left[\frac{2m}{\hbar^2}(E_n-U(y))\right]^{\frac{1}{2}}dy, \tag{30a}$$

$$\beta_{nc}(x)=\int_x^0[-\gamma(y)]^{\frac{1}{2}}dy, \tag{30b}$$

by the use of the two implicit equations,

$$\begin{aligned} \beta_c(x)&=\int_{\frac{1}{2}}^z\left[1-\frac{1}{4z^2}\right]^{\frac{1}{2}}dz=z\left[1-\frac{1}{4z^2}\right]^{\frac{1}{2}}-\tfrac{1}{2}\arcsin\left[1-\frac{1}{4z^2}\right]^{\frac{1}{2}} \\ &=z\left[1-\frac{1}{4z^2}\right]^{\frac{1}{2}}-\tfrac{1}{2}\arccos\left(\frac{1}{2z}\right), \end{aligned} \tag{31a}$$

$$\beta_{nc}(x)=\int_z^{\frac{1}{2}}\left[\frac{1}{4z^2}-1\right]^{\frac{1}{2}}dz=\tfrac{1}{2}\ln\left[\frac{1+(1-4z^2)^{\frac{1}{2}}}{2z}\right]-\tfrac{1}{2}(1-4z^2)^{\frac{1}{2}} \tag{31b}$$

for $z\geq\frac{1}{2}$ or $z\leq\frac{1}{2}$, respectively.

For the classical region, we find

$$z=Q[1-\tfrac{1}{8}Q^{-2}-(7/384)Q^{-4}-(83/15\,360)Q^{-6}+\cdots], \quad (32a)$$

$$Q\equiv\beta_c(x)+\tfrac{1}{4}\pi, \quad (32a')$$

which, even at the turning point, $\beta=0, Q=\frac{1}{4}\pi$, gives $z=0.56$ instead of the exact $z=z^{(0)}=\frac{1}{2}$. One has, with $dQ/dx=\gamma^{\frac{1}{2}}$,

$$dz/dx=z_1=\gamma^{\frac{1}{2}}[1+\tfrac{1}{8}Q^{-2}+(7/128)Q^{-4}+(83/3072)Q^{-6}+\cdots]. \quad (32a'')$$

For the nonclassical region, one obtains

$$z=e^{-\Omega}[1+e^{-2\Omega}+3e^{-4\Omega}+(37/3)e^{-6\Omega}+\cdots], \quad (32b)$$

$$\Omega\equiv 2\beta_{nc}(x)+1, \quad (32b')$$

$$dz/dx=z_1=2(-\gamma)^{\frac{1}{2}}e^{-\Omega}\times[1+3e^{-2\Omega}+15e^{-4\Omega}+(259/3)e^{-6\Omega}+\cdots]. \quad (32b'')$$

The approximation of (32b) gives $z=0.45$ at the turning point.

For the region of the turning point, we write

$$\beta_c=\int_0^x\gamma^{\frac{1}{2}}dy=\int_0^x\gamma^{\frac{1}{2}}(d\gamma/dy)^{-1}d\gamma,$$

and integrate by parts repeatedly to obtain,

$$\beta=\frac{2}{3}\frac{|\gamma|^{\frac{3}{2}}}{\gamma_1}[1+F(\gamma)] \quad (33)$$

$$F(\gamma)=\frac{2}{5}\gamma\frac{\gamma_2}{\gamma_1^2}+\frac{4}{35}\gamma^2\left[3\frac{\gamma_2^2}{\gamma_1^4}-\frac{\gamma_3}{\gamma_1^3}\right]+\frac{8}{315}\gamma^3\left[15\frac{\gamma_2^3}{\gamma_1^6}-10\frac{\gamma_2\gamma_3}{\gamma_1^5}+\frac{\gamma_4}{\gamma_1^4}\right]+\frac{16}{3465}\gamma^4\left[105\frac{\gamma_2^4}{\gamma_1^8}-105\frac{\gamma_2^2\gamma_3}{\gamma_1^7}+10\frac{\gamma_3^2}{\gamma_1^6}+\frac{15\gamma_2\gamma_4}{\gamma_1^6}-\frac{\gamma_5}{\gamma_1^5}\right]. \quad (33')$$

Equation (33) with the absolute value of γ is valid for both β_c and β_{nc}; however, the algebraic values are to be used in $F(\gamma)$. The expansions for z and z_1 then come out in a simple power series of $(6\beta_c)^{\frac{2}{3}}$ for $x>0$ and of $-(6\beta_{nc})^{\frac{2}{3}}$ for $x<0$. The equations, after a great quantity of algebraic manipulation of (31a) and (31b), become

$$z=\tfrac{1}{2}+(2\gamma_1)^{-\frac{2}{3}}\gamma(1+F)^{\frac{2}{3}}+\tfrac{3}{5}(2\gamma_1)^{-4/3}\gamma^2(1+F)^{4/3}-\frac{2}{175}(2\gamma_1)^{-2}\gamma^3(1+F)^2-\frac{479}{7875}(2\gamma_1)^{-8/3}\gamma^4(1+F)^{8/3}+\frac{140\,178}{336\,875}(2\gamma_1)^{-10/3}\gamma^5(1+F)^{10/3}+\cdots \quad (34)$$

$$(dz/dx)=z_1=\tfrac{1}{2}(2\gamma_1)^{\frac{1}{3}}(1+F)^{-\frac{1}{3}}\left[1+\frac{6}{5}(2\gamma_1)^{-\frac{2}{3}}\gamma(1+F)^{\frac{2}{3}}-\frac{6}{175}(2\gamma_1)^{-\frac{4}{3}}\gamma^2(1+F)^{\frac{4}{3}}-\frac{1916}{7875}(2\gamma_1)^{-2}\gamma^3(1+F)^2+\frac{140\,178}{67\,375}(2\gamma_1)^{-8/3}\gamma^4(1+F)^{8/3}+\cdots\right]. \quad (34')$$

It is clear that the equations are valid only for nonzero $\gamma_1=d\gamma/dx=-(2m/\hbar^2)dU/dx$. If the second and higher derivatives of $U(x)$ are identically zero the functional, $F(\gamma)$, is zero, and $\gamma=\gamma_1 x$ gives

$$z=\tfrac{1}{2}[1+(2\gamma_1)^{\frac{1}{3}}x+\tfrac{3}{10}(2\gamma_1)^{\frac{2}{3}}x^2+\cdots]. \quad (34'')$$

For nonzero γ_1, the Schrödinger solution,

$$\psi(x)=z_1^{-\frac{1}{2}}\sin z(x),$$

goes smoothly through the turning point.

5. HIGHER ORDER SOLUTIONS

The higher order solutions are to be obtained from (24) by replacing the $\gamma(x)=(2m/\hbar^2)[E_n-U(x)]$ occurring in the last section by $(2m/\hbar^2)(E_n-U)+q(z^{(\nu)})$, with $z^{(\nu)}$ the solution of one lower order. However, the limit of integration over x is now chosen at that value of x for which the new $\gamma(x)$ is zero, and the two integrals $\beta_c(x)$ and $\beta_{nc}(x)$ of Eq. (30) are evaluated from this new origin of x.

One may conveniently use the second expression of Eq. (25) for the operator $q(z)$ with the three equations, (32a), (32b), or (34) to find the new $\gamma(x)$ in terms of that of lower order. The equations obtained from the first two for $\gamma^{(1)}$ are

$$\gamma^{(1)}=\gamma\left[1-\frac{1}{4}\frac{\gamma_2}{\gamma^2}+\frac{5}{16}\frac{\gamma_1^2}{\gamma^3}-\frac{1}{4}Q^{-2}-\frac{1}{2}Q^{-4}-\frac{25}{48}Q^{-6}+\cdots\right], \quad (35a)$$

$$\gamma^{(1)}=\gamma\left[1-\frac{1}{4}\frac{\gamma_2}{\gamma^2}+\frac{5}{16}\frac{\gamma_1^2}{\gamma^3}+16e^{-2\Omega}+240e^{-4\Omega}+2672e^{-6\Omega}+\cdots\right], \quad (35b)$$

for the classical and nonclassical regions, respectively. If, in turn, $\gamma^{(1)}$ and the corresponding $Q^{(1)}$ or $\Omega^{(1)}$ are used in the right hand side, the expressions give $\gamma^{(2)}$, etc. For the region of the turning point, one has

$$\gamma^{(1)}=\left[\frac{1}{35}(2\gamma_1)^{\frac{4}{3}}-\frac{1}{14}\frac{\gamma_3}{\gamma_1}+\frac{9}{140}\left(\frac{\gamma_2}{\gamma_1}\right)^2\right]+\gamma\left[\frac{67}{75}-\frac{4}{525}(2\gamma_1)^{\frac{4}{3}}\frac{\gamma_2}{\gamma_1^2}+\frac{1}{63}\frac{\gamma_4}{\gamma_1^2}+\frac{32}{525}\frac{\gamma_2^3}{\gamma_1^4}-\frac{23}{315}\frac{\gamma_2\gamma_3}{\gamma_1^3}\right]+O(\gamma^2). \quad (36)$$

In the case that all derivatives of U higher than the first are zero, $\gamma_2=\gamma_3=\cdots=0$, one has $\gamma=\gamma_1 x$ and the zero of $\gamma^{(1)}$ is now at

$$x^{(1)}[\gamma^{(1)}=0]=-\frac{30}{469}(2\gamma_1)^{-\frac{1}{3}}. \qquad (36')$$

Using this in (34″), we see that, whereas $z^{(0)}$ is $\frac{1}{2}(1-30/469)$ at this value of x for this case, the first order $z^{(1)}$ will take its boundary condition value of exactly one-half. Thus the first and zeroth-order values of z at the turning point differ by less than 10% for this case of constant dU/dx.

6. GENERAL SOLUTION FOR z

Finally we wish to discuss briefly the most general solution of Eq. (11) for z, which, even with a fixed boundary condition, such as the one which we employed $z\to 0$, $x\to -\infty$, does not uniquely determine the function $z(x)$.

Plaskett,[7] using a method due to Milne,[8] has obtained a general solution for z_1 in (14) by considering the Wronskian, W, of two independent solutions, ψ_1 and ψ_2, of the Schrödinger equation. Of these, only one can be taken as an eigenfunction. The Wronskian is defined as

$$W=\psi_2(d\psi_1/dx)-\psi_1(d\psi_2/dx), \qquad (37)$$

and is a nonzero constant.[9] By defining

$$s(x)=(\psi_1^2+\psi_2^2)^{\frac{1}{2}}, \qquad (38)$$

one can verify from (1) and (37) that

$$-\frac{1}{s}(d^2s/dx^2)+\frac{W^2}{s^4}=\gamma. \qquad (39)$$

Hence, by (14), z_1 can be identified as

$$z_1=W/(\psi_1^2+\psi_2^2). \qquad (40)$$

Commenting on this derivation, Ballinger and March[10] suggest that z_1 cannot be determined uniquely by (40) since if ψ_2 is a solution of (1), then so is $c\psi_2$ with c an arbitrary constant. They would write a more general function Z_1:

$$Z_1=cW/(\psi_1^2+c^2\psi_2^2), \qquad (41)$$

$$Z_1=z_1,\quad c=1, \qquad (42)$$

We now show that this is no more than a formal difficulty and that aside from normalization the most general form $[Z_1^{-\frac{1}{2}}\sin Z]$ is the same function $[z_1^{-\frac{1}{2}}\sin z]$. Let $(d^2\psi_1/dx^2)+\gamma\psi_1=0$ and $(d^2\psi_2/dx^2)+\gamma\psi_2=0$ so that, if z_1 is a particular solution of (14), we have two independent solutions:

$$\psi_1=z_1^{-\frac{1}{2}}\sin z;\quad \psi_2=z_1^{-\frac{1}{2}}\cos z. \qquad (43)$$

ψ_1 is an allowed function of the type (15). ψ_2 will not go to zero at $x=-\infty$, and does not obey the boundary condition. The Wronskian of these is $+1$ by Eq. (37). Inserting into Eq. (41), we obtain

$$Z_1=\frac{cz_1}{(c^2-1)\cos^2 z+1}, \qquad (44)$$

$$Z=\int_{-\infty}^{x}Z_1dx=\int_0^z\frac{cdz}{(c^2-1)\cos^2 z+1}$$
$$=\tfrac{1}{2}\arctan\left[\frac{2c\sin z\cos z}{c^2\cos^2 z-\sin^2 z}\right]. \qquad (45)$$

From (45), we have

$$Z_1=\frac{cz_1}{(c^2-1)\cos^2 z+1}. \qquad (46)$$

The trigonometric relations,

$$\sin[\tfrac{1}{2}(\arctan\theta)]=[\tfrac{1}{2}-\tfrac{1}{2}\cos(\arctan\theta)]^{\frac{1}{2}},$$
$$\cos(\arctan\theta)=(1+\theta^2)^{-\frac{1}{2}},$$

combined with (45), lead to

$$\sin Z=\frac{\sin z}{[(c^2-1)\cos^2 z+1]^{\frac{1}{2}}}. \qquad (47)$$

Then the most general eigenfunction would be

$$\psi=Z_1^{-\frac{1}{2}}\sin Z=c^{-\frac{1}{2}}z_1^{-\frac{1}{2}}\sin z. \qquad (48)$$

This is seen to be the same function as (15), since neither function is normalized as written. The different c's can be of no real significance, because they will be "washed out" in the normalization.

---

[7] J. S. Plaskett, Proc. Phys. Soc. (London) **A66**, 178 (1953).
[8] W. E. Milne, Phys. Rev. **35**, 863 (1930).
[9] See any book on differential equations.
[10] R. A. Ballinger and N. H. March, Proc. Phys. Soc. (London) **A67**, 378 (1954).