Approximate Solutions to the One-Dimensional Schrödinger Equation by the Method of Comparison Equations*

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(Received 13 December 1972)

The method of "comparison equations" for obtaining approximate solutions to the one-dimensional Schrödinger equation is discussed. In this method, one Schrödinger equation, $\psi''(x) + k^2(x)\psi(x) = 0$, is transformed into another, $v''(z) + K^2(z)v(z) = 0$, by a simultaneous change of independent and dependent variables, $x \to z$, $\psi \to v$. Then $\psi(x)$ and $v(z)$ are related by $\psi(x) = v(z)(dz/dx)^{-(1/2)}$ whenever $k^2(x)$ and $K^2(z)$ satisfy the relation $K^2(z)(dz/dx)^2 = k^2(x) - (1/2)\langle z;x\rangle$. Here $\langle z;x\rangle = z'''/z' - (3/2)(z''/z')^2$ is the Schwarzian derivative of z with respect to x and the prime indicates d/dx. A set of "best" criteria for the transformed potential $K^2(z)$ is obtained, where by "best" is meant that we can completely neglect $\langle z;x\rangle$ in first approximation and yet not have the turning-point problems that plague the WKB method (which is a special case of the comparison-equation method). The WKB method sets $K^2(x) \equiv 1$ and neglects $\langle z;x\rangle$; the result is that the transformation $x \to z$, $\psi \to v$ is singular at the turning points, where $k^2(x) = 0$. We choose $K^2(z)$ to have the proper asymptotic behavior far from the turning points, so that $z' \approx 1$; hence $\langle z;x\rangle \approx 0$ in these regions, and we match the zeroes of $k^2(x)$ and $K^2(z)$ in order to keep the transformation regular. This method is applied to various potentials with one and two turning points. Transmission and reflection coefficients T and R and transmitted and reflected phase shifts μ and ν are calculated for potentials with one turning point and potential barriers, and expressed in terms of the energy E and the quantity $W = |\int_{x_1}^{x_2} k\,dx|$, where $x_{1,2}$ are the possibly complex turning points, $k^2(x_{1,2}) = 0$. Quantization rules, in terms of the classical action, are derived for various types of potential wells.

I. INTRODUCTION

In the last decade there has been a great revival of interest in semiclassical methods of obtaining approximate solutions to the Schrödinger equation (see Ref. 1 for a comprehensive survey). A good deal of this attention has been directed at so-called "extensions" of the WKB method, which aim at finding uniform approximations by the method of comparison equations.[2,3] The phrase "so-called" is used because these "extensions" are really special cases of a powerful general technique available for a long time,[4,5] as is the WKB method.

This technique relies on an equivalence between any two second-order linear differential equations. Any such equation may by a simple substitution be brought into the form of the one-dimensional Schrödinger equation, so we consider only the Schrödinger equation. Writing $d^2\psi(x)/dx^2 = \psi''(x)$, $d^2v(z)/dz^2 = v''(z)$, and $dz/dx = z'$, a little algebra shows that any two one-dimensional Schrödinger equations[6]

$$\psi''(x) + k^2(x)\psi(x) = 0, \tag{1}$$

$$v''(z) + K^2(z)v(z) = 0 \tag{2}$$

are equivalent, in the sense that the solutions ψ and v to (1) and (2) are related by

$$\psi(x) = v(z)/(z')^{1/2} \tag{3}$$

whenever $z(x)$ satisfies the relation

$$(z')^2 K^2(z) = k^2(x) - \tfrac{1}{2}\langle z;x\rangle, \tag{4}$$

where

$$\langle z;x\rangle = \frac{z'''}{z'} - \frac{3}{2}\left(\frac{z''}{z'}\right)^2 \tag{5}$$

is the Schwarzian derivative[7] of z with respect to x.

{Note that a graph of $k^2(x) = (2m/\hbar^2)[E - V(x)]$ or $K^2(z)$ looks upside down, being essentially the negative of $V(x)$ (shifted up or down, depending on the sign of E). Thus, for instance, a concave-upward K^2 is really a potential barrier, even though it *looks* like a well. This can be confusing, but it is done as a matter of universal convention and enables us to write $S(x) = \int k\,dx$ in classical regions and $\int |k|\,dx$ in nonclassical regions, instead of vice versa.}

Thus, if we know the solutions to any one-dimensional Schrödinger equation, say (2), then we may obtain the solutions to any other, say (1), by solving (4) for $z(x)$ and using (3). Of course, (4) is a nonlinear third-order equation and hence not generally solvable in closed form. But (4) *is* readily solved if $\langle z;x\rangle$ is zero. Then integration yields the implicit equation

$$\int_{z_0}^{z} K(z)\,dz = \int_{x_0}^{x} k(x)\,dx \tag{6}$$

for $z(x)$, where $z_0 \equiv z(x_0)$. If $\langle z;x\rangle$ is not zero, but small, then (6) is the first step in some iterative scheme for solving (4) for $z(x)$.

There are two such schemes available to us. The first, due to Hecht and Mayer,[8] consists of choosing $K^2(z)=1$, so that the solutions $v(z)$ of (2) are particularly simple, namely, $\sin z$ and $\cos z$. They then develop an iteration scheme for solving (4) for $z(x)$. For certain potentials and under certain conditions, they are able by this method to calculate $z(x)$, and hence $\psi(x)$, to any desired degree of accuracy.

This method has certain disadvantages, though. First, it needs considerable modification to apply it to potentials with more than one turning point, and it breaks down if $[k^2(x)]' = -(2m/\hbar^2)V'(x)$ equals zero. Second, in order to obtain quantities of interest such as the transmission and reflection coefficients and phase shifts (T, R, μ, ν, defined at the end of this section), one must calculate integrals of the type

$$\int [k^2(x) - \tfrac{1}{2}\langle z; k\rangle]^{1/2} dx,$$

where one or both of the limits of integration are the classical turning points, $k^2(x)=0$. In this scheme there is no handle on how small $\langle z; x\rangle$ is; hence we cannot neglect it, particularly near the turning points. These integrals are therefore very difficult to perform.

The second method, developed by Fröman and Fröman,[9] consists in setting $z'(x)$ equal to some convenient function $q(x)$, usually but not always chosen to be $k(x)$. Then from (4) we have

$$K^2(z) = 1 + \frac{k^2 - q^2}{q^2} - \frac{\langle z; x\rangle}{2q^2}.$$

It is then assumed that the last two terms on the right-hand side of this equation are small compared to 1, (2) is converted to an integral equation, and an iteration scheme based on the solutions $e^{\pm iz}$ of (2) with $K^2=1$ is developed. This is a rigorous WKB method and suffers from the same difficulties that the more prosaic WKB approach suffers. That is, the turning points $k^2(x)=0$ manifest themselves in the unpleasant fashion of essential singularities in the WKB wave function, so that the Stokes phenomenon makes the problem of connection formulas very difficult.[10] It proves to be impossible using this method to calculate the phase shifts μ and ν in lowest order.

Both of these methods suffer from essentially the same difficulty: one chooses $K^2(z)$ [or $z(x)$] to be simple; the intent is to make (2) [or (4)] elementary in order to facilitate an iteration scheme. However, what we should really do to make the iteration scheme easier is to make $\langle z; x\rangle$ small, so that we can justify taking the iteration scheme to lowest order only, i.e., justify ignoring $\langle z; x\rangle$ altogether.

We want to be able to pick $K^2(z)$ so that (a) $v'' + K^2 v = 0$ is a known equation with known solutions; (b) $K^2(z)$ admits a solution $z(x)$ to (4) which is approximately linear in x, $z' \approx$ constant; hence $\langle z; x\rangle$ is small and we ignore it; and (c) z' is finite (nonzero and noninfinite) everywhere; hence there are no Stokes phenomenon and connection-formula problems. Then z and x are (approximately) related by (6) and ψ and v by (3).

Condition (c) means that we demand that if $z(x)$ is calculated by (6), and x_0 is a root (or singularity) of $k^2(x)$, then $z_0 \equiv z(x_0)$ is a root (or singularity) of $K^2(z)$ and vice versa. That is, $\psi'' + k^2\psi = 0$ and $v'' + K^2 v = 0$ have corresponding turning points and singularities. This may be done trivially for one turning point—it is just a matter of having the origin of z in the proper place. For more than one turning point, as will be illustrated later, $K^2(z)$ must also be a function of one or more parameters α, $K^2 = K^2(z; \alpha)$, which must then be adjusted generally as a function of energy to ensure that the turning points x_0 and z_0 of the original and transformed equations correspond [$z_0 \equiv z(x_0)$] for *all* energies. In addition, for potential wells with a finite number of bound states, an extra parameter is necessary to ensure that the transformed equation has the same number of bound states as the original one. These α will, in general, then depend on the energy E and hence the transformation $x \to z$, $\psi \to v$ will be energy dependent. The result is that z', the Jacobian of the transformation $z \to x$, is finite; the transformation $z \to x$ is regular; and $\psi(x)$ is regular through the turning points.

The obvious question to be asked is: Can we always, for an arbitrary $k^2(x)$, find a $K^2(z)$ which meets the requirements (a)–(c) with the Schwarzian derivative $\langle z; x\rangle$ small enough so that the approximation of ignoring it is good everywhere? The answer is not known, but is probably yes for any case of interest. For instance (Fig. 1), suppose the potential $V(x)$ in $k^2 = (2m/\hbar^2)[E - V(x)]$ is a barrier of height V_0 and $V(\pm\infty)=0$. Then we pick a $K^2(z)$ of similar shape as $k^2(x)$, $K^2(z) = (2m/\hbar^2)$

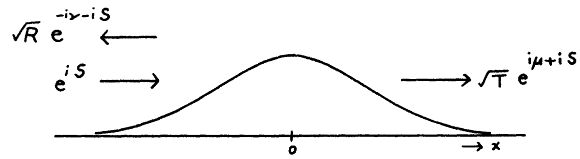

FIG. 1. A potential barrier with $V(+\infty) = V(-\infty) = 0$. We typically seek a wave function which has the asymptotic behavior of an incoming wave and a scattered wave, $\exp[iS(x)] + R^{1/2}\exp[-i\nu - iS(x)]_{x \to -\infty} \sim \psi(x)_{x \to +\infty} \sim T^{1/2} \times \exp[i\mu + iS(x)]$. Phases are measured from the left and right turning points for $E \le V_{max}$ and from x_0 such that $V(x_0) = V_{max}$ for $E \ge V_{max}$.

$\times(E - V_0 \operatorname{sech}^2 \gamma z)$, with γ a parameter to be determined. Then for large $|x|$, Eq. (4) becomes

$$(2mE/\hbar^2)(z')^2 = (2m/\hbar^2)E - \tfrac{1}{2}\langle z; x\rangle,$$

which manifestly has a solution z' = constant for large $|x|$. Hence conditions (a) and (c) are met, and (b) is met for large $|x|$. We may not so safely be able to ignore $\langle z; x\rangle$ for *all* x, but at least $\psi(x)$ obtained by doing so is regular. This removes the most troublesome features of the WKB methods. Furthermore, the calculations of Miller and Good[2] on two turning points show that in this case the approximate wave function is very accurate throughout the entire range of x.

The procedure then is the following. Pick a $K^2(z)$ so that (i) $v'' + K^2 v = 0$ is a known equation with known solutions, (ii) Eq. (4) admits a solution $z(x)$ which is linear in x in asymptotic regions (e.g., $|x| \gg 1$ for a potential barrier), (iii) the turning points in $K^2(z)$ and $k^2(x)$ may be matched. (iv) Calculate $z(x)$ from Eq. (6):

$$\int^z K(z)\,dz = \int^x k(x)\,dx.$$

(v) Obtain $\psi(x)$ from Eq. (3):

$$\psi(x) = v(z)/\sqrt{z'}.$$

Because this approximate wave function is valid through the turning points, the difficulties with the connection formulas and the Stokes phenomenon do not arise, and expressions for the reflection and transmission coefficients R and T and the reflected and transmitted phase shifts ν and μ are easily obtained. By choosing K^2 to have nearly the same functional dependence on z as k^2 has on x, we make z' be nearly constant; hence $\langle z; x\rangle$, which contains higher derivatives of z in every term, is made small. This is in stark contrast to the WKB method, which chooses K^2 constant instead of z'' small, that is, the approximate ψ simple instead of accurate.

In asymptotic regions, e.g. $|x| \gg 1$ for a potential barrier, we define the transmission and reflection coefficients T and R and the phase shifts μ and ν of the transmitted and reflected waves by specifying the boundary conditions to be that, for $x \to \infty$, the wave function shall be a transmitted wave traveling to the right (see Fig. 1):

$$\psi(x) \underset{x\to+\infty}{\sim} T^{1/2}\exp(i\mu)\exp\left(+i\int_{x_2}^{x} k\,dx\right), \tag{7a}$$

where x_2 is the right-hand turning point. For $x \to -\infty$, ψ consists of an incoming (from $-\infty$) wave of coefficient 1 and a reflected, outgoing wave (Fig. 1):

$$\psi(x) \underset{x\to-\infty}{\sim} \exp\left(+i\int_{x_1}^{x} k\,dx\right) + R^{1/2}\exp(-i\nu)\exp\left(-i\int_{x_1}^{x} k\,dx\right), \tag{7b}$$

where x_1 is the left-hand turning point.

We shall focus our attention on finding expressions for T, R, μ, and ν in terms of E and the potential $V(x)$ for scattering problems and quantization rules for potential wells. In Secs. II–IV we deal with problems with one and two turning points.

Unless otherwise stated, all special functions we use are given in the notation of Abramowitz and Stegun (AS).[11]

II. ONE TURNING POINT

By one turning point we mean that, for *each* value of E, there is *at most* one value of x, called the turning point and denoted by x_t, for which $k^2 = (2m/\hbar^2)[E - V(x_t)] = 0$. Above some E there may be no turning point. Hence $V(x)$ and $k^2(x)$ are monotonic functions of x. For definiteness we suppose that $V(x)$ is monotonic decreasing, hence k^2 monotonic increasing, for x increasing. The region of the x axis $x \le x_t$, where $k^2 \le 0$, is the nonclassical region; the region $x \ge x_t$, where $k^2 \ge 0$, is the classical region. The corresponding regions of the z axis are $z \le z_t$, $K^2 \le 0$, the nonclassical region and $z \ge z_t$, $K^2 \ge 0$, the classical region.

We define

$$S_{\mathrm{NC}}(x) = \int_{x_t}^{x} |k|\,dx = \int_{z_t}^{z} |K|\,dz \le 0 \tag{8}$$

in the nonclassical region and

$$S_{\mathrm{CL}}(x) = \int_{x_t}^{x} k\,dx = \int_{z_t}^{z} K\,dz \ge 0 \tag{9}$$

in the classical region. In both regions,

$$S'(x) = \frac{d}{dx}S(x) = |k(x)| = z'\,|K(z)| \ge 0. \tag{10}$$

We seek an approximate solution to the Schrödinger equation which has the form of an incoming wave (from $x = +\infty$, hence traveling to the left) with coefficient unity and a reflected outgoing wave with coefficient $R^{1/2}e^{-i\nu}$ for $x \gg 1$. Hence we seek a ψ such that

$$\psi(x) \underset{x\to+\infty}{\sim} e^{-iS_{\mathrm{CL}}(x)} + R^{1/2}e^{-i\nu}e^{+iS_{\mathrm{CL}}(x)}. \tag{11}$$

Here R is the reflection coefficient and ν is the phase shift of the reflected wave.

$\psi(x)$ must also satisfy appropriate boundary conditions at the left end of its domain of definition. If $V(x)$ is bounded, we demand that for $E > V_{\max}$,

$$\psi(x) \underset{x\to-\infty}{\sim} T^{1/2}e^{i\mu}e^{-iS_{\mathrm{CL}}(x)}, \tag{12}$$

where T is the transmission coefficient and μ is the phase shift of the transmitted wave. If $V(x)$

$\to\infty$ as $x\to-\infty$, we demand that ψ be zero at minus infinity, $\psi(-\infty)=0$. If $V(x)$ is infinite at some finite x, say at $x=0$, we demand that $\psi(0)V(0)$ be finite; hence $\psi(0)=0$ (and goes fast enough to zero).

We will discuss three types of potentials: cases (A), (B), and (C). For case (A),

$$\text{(A)}\quad V(\mp\infty)=\pm\infty,\quad -\infty\leqslant x\leqslant+\infty.$$

We assume that the energy scale has been adjusted so that $V(0)=0$. Note that $-\infty\leqslant E\leqslant\infty$. We then choose

$$\text{(A)}\quad K^2(z)=E+z/\beta. \tag{13}$$

Thus $-\infty\leqslant z\leqslant\infty$, $K^2(\pm\infty)=k^2(\pm\infty)=\pm\infty$, and $z_t=-\beta E$. [We use the symbols E and V for energy multiplied by $2m/\hbar^2$; they are therefore of dimension (length)$^{-2}$, so that β is a positive constant of dimension (length)$^{+3}$.] For case (B),

$$\text{(B)}\quad V(0)=+\infty,\quad V(\infty)=0,\quad 0\leqslant x\leqslant+\infty.$$

Here $E\geqslant0$. We then choose two examples for K^2:

$$\text{(B1)}\quad K^2(z)=E-a^2/z^2, \tag{14}$$

$$\text{(B2)}\quad K^2(z)=E-2a/z. \tag{15}$$

Thus in both cases $0\leqslant z\leqslant\infty$, $K^2(\infty)=k^2(\infty)=E$, and $z_t=a/E^{1/2}$ for (B1) and $z_t=2a/E$ for (B2). [Again, a is a positive constant, dimensionless for (B1) and of dimension (length)$^{-1}$ for (B2).] For case (C),

$$\text{(C)}\quad |V(\pm\infty)|<\infty,\quad -\infty\leqslant x+\infty.$$

We assume the energy scale has been adjusted so that $V(-\infty)=-V(+\infty)=V_0$. We have $E\geqslant-V_0$ and we choose

$$\text{(C)}\quad K^2(z)=E+V_0\tanh(z/\beta). \tag{16}$$

Thus $-\infty\leqslant z\leqslant\infty$, $K^2(\pm\infty)=k^2(\pm\infty)=E\pm V_0$, and $z_t=-\beta\tanh^{-1}(E/V_0)$. ($\beta$ is a positive constant of dimension length.)

Case (A) is the Langer approximation[12]; (B1) is the case treated by Hecht and Mayer[8] and is the same as the radial wave equation for three-dimensional scattering by a constant (here zero) potential. Case (B2) yields the $l=0$ radial wave equation for three-dimensional scattering by a repulsive Coulomb potential. The reason we give two examples for the type (B) is the boundary condition at $x=0$. Precisely how fast $V(x)$ approaches infinity as x approaches zero matters; hence it matters how well we tailor the transformed $K^2(z)$ to the original $k^2(x)$. As we shall see, the phase shift ν differs considerably depending on the power with which $K^2(z)$ diverges at zero. Case (C) is a smooth "step" potential, rising from $-V_0$ to V_0 as a particle strikes it from the right. All four potentials and $K^2(z)$ are graphed in Fig. 2.

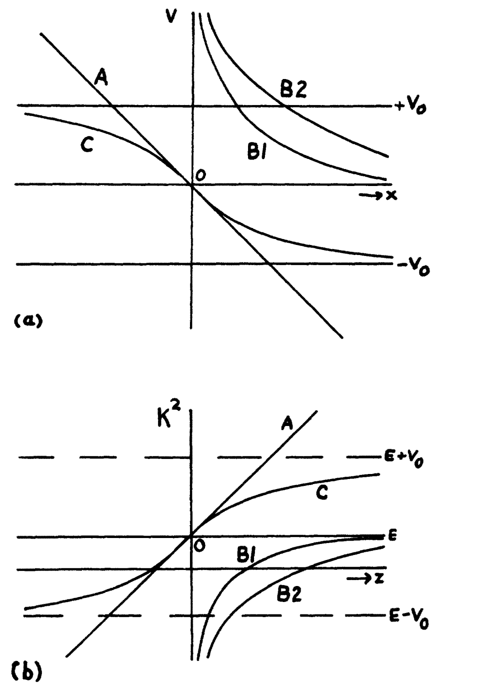

FIG. 2. $V(x)$ and $K^2(z)$ for the one-turning-point problems, (a) $V(x)$, (b) $K^2(z)$. (A) $K^2(z)=E+z/\beta$, (B1) $K^2(z)=E-a^2/z^2$, (B2) $K^2(z)=E-2a/z$, and (C) $K^2(z)=E+V_0\tanh(z/\beta)$.

In each case we follow the same format. First, $S(x)$ and $(z')^{-1/2}$ and their asymptotic behavior are given. Then the solution $\psi(x)$ with the proper asymptotic form and/or boundary condition is presented and hence expressions for R and ν (and T, μ) are obtained. Most, if not all, detailed calculations are omitted; reference is made to the appropriate sections in AS.

For case (A), where $K^2(z)=E+z/\beta$,

$$\begin{aligned}
&z_t=-\beta E,\quad -\infty\leqslant E\leqslant\infty\\
&S_{\rm CL}(x)=\tfrac{2}{3}\beta(E+z/\beta)^{3/2},\\
&S_{\rm NC}(x)=-\tfrac{2}{3}\beta|E+z/\beta|^{3/2},\\
&(z')^{-1/2}=(S')^{-1/2}|E+z/\beta|^{1/4},\\
&v(z)=\mathrm{Ai}(-\tfrac{2}{3}\beta(E+z/\beta)^{3/2}).
\end{aligned} \tag{17}$$

See AS, Sec. 10.4, p. 446ff, for the Airy functions. The other Airy function Bi, being singular at $-\infty$, does not satisfy the boundary conditions.

Hence $\psi(x)$ goes exponentially to zero as $x\to-\infty$ (remember $S_{\rm NC}<0$):

$$\psi(x)\underset{x\to-\infty}{\sim}(2\pi\beta^{1/3}S')^{-1/2}e^{S_{\rm NC}(x)}.$$

As $x\to+\infty$, $\psi(x)$ goes asymptotically as

$$\psi(x)\underset{x\to+\infty}{\sim}(\pi\beta^{1/3}S')^{-1/2}\sin[S(x)+\tfrac{1}{4}\pi].$$

Hence

$$R=1, \quad \nu=\tfrac{1}{2}\pi. \tag{18}$$

[We have used $\sin(S+\phi)=\frac{1}{2}i\, e^{-i\phi}(e^{-iS}+e^{-i(\pi-2\phi)}\times e^{+iS})$; hence $\nu=\pi-2\phi$. Here $\phi=\frac{1}{4}\pi$; so $\nu=\frac{1}{2}\pi$.]

For case (B1), where $K^2(z)=E-a^2/z^2$,

$$z_t=a/\sqrt{E}, \quad 0\leq E$$

$$S_{\rm CL}(x)=(Ez^2-a^2)^{1/2}-a\sin^{-1}\left(1-\frac{a^2}{Ez^2}\right)^{1/2} \underset{x\to+\infty}{\sim} z\sqrt{E}-\tfrac{1}{2}a\pi,$$

$$S_{\rm NC}(x)=(a^2-Ez^2)^{1/2}+a\ln\left(\frac{a+(a^2-Ez^2)^{1/2}}{z\sqrt{E}}\right) \underset{x\to 0}{\sim} a\ln(e\,zE^{1/2}/a),$$

$$(z')^{-1/2}=(S')^{-1/2}(E-a^2/z^2)^{1/4} \underset{x\to+\infty}{\sim} (S'_{\rm CL})^{-1/2}E^{1/4}\sim 1 \quad \underset{x\to 0}{\sim} (S'_{\rm NC})^{-1/2}(a/z)^{1/2},$$

$$v(z)=E^{1/4}z^{1/2}J_\rho(z\sqrt{E}), \tag{19}$$

where $\rho=+(a^2+\frac{1}{4})^{1/2}$. See AS, Chap. 9, Eqs. 9.1.7 and 9.2.1, for the Bessel function J_ρ. The other Bessel function Y_ρ is irregular at $z=0$ and is therefore discarded.

Thus $\psi(0)=0$ and

$$\psi(x)\underset{x\to+\infty}{\sim}(2/\pi)^{1/2}\cos[S(x)-\tfrac{1}{4}\pi-\phi],$$

where

$$\phi=\tfrac{1}{2}\pi(\rho-a)=\tfrac{1}{2}\pi[(a^2+\tfrac{1}{4})^{1/2}-a].$$

Hence

$$R=1, \quad \nu=\tfrac{1}{2}\pi+2\phi=\tfrac{1}{2}\pi[1+(a^2+\tfrac{1}{4})^{1/2}-a]. \tag{20}$$

Note that, as in (A), ν is independent of the energy E. This is expected in both cases, since in (A) a change in E is just a translation of the z axis, and in (B1) we have the $V(x)\equiv 0$ radial wave equation; so in neither case do we expect ν or R to depend on E.

For case (B2), where $K^2=E-2a/z$,

$$z_t=2a/E, \quad 0\leq E$$

$$S_{\rm CL}(x)=[z(Ez-2a)]^{1/2}-\frac{2a}{\sqrt{E}}\tanh^{-1}\left(1-\frac{2a}{Ez}\right)^{1/2} \underset{x\to+\infty}{\sim} z\sqrt{E}+\frac{a}{\sqrt{E}}\ln\left(\frac{a}{2zeE}\right),$$

$$S_{\rm NC}(x)=[z(2a-Ez)]^{1/2}+\frac{a}{\sqrt{E}}\sin^{-1}\left(\frac{E^{1/2}}{a}[z(2a-Ez)]^{1/2}\right),$$

$$(z')^{-1/2}=(S')^{-1/2}|E-2a/z|^{1/4} \underset{x\to+\infty}{\sim}(S'_{\rm CL})^{-1/2}E^{1/4}\approx 1 \quad \underset{x\to 0}{\sim}(S'_{\rm NC})^{-1/2}(2a/z)^{1/4},$$

$$v(z)=F_0(a/\sqrt{E}, z\sqrt{E}). \tag{21}$$

See AS, Chap. 14, Eqs. 14.1.3–7, Sec. 14.5, for the Coulomb wave functions F_0 and G_0. The latter is irregular at $z=0$; hence it is discarded.

Then $\psi(0)=0$ and

$$\psi(x)\underset{x\to+\infty}{\sim}\sin[S(x)+\phi-(a/\sqrt{E})\ln(a/e\sqrt{E})],$$

where

$$\phi=\arg\Gamma(1+ia/\sqrt{E}).$$

Hence

$$R=1, \quad \nu=\pi-2\arg\Gamma(1+ia/\sqrt{E})+(2a/\sqrt{E})\ln(a/e\sqrt{E}). \tag{22}$$

ν is plotted as a function of E in Fig. 3(a).

For case (C), where $K^2(z)=E+V_0\tanh(z/\beta)$, there are two distinct energy intervals to consider. They are $E/V_0\equiv\alpha$ greater than and less than one. For $\alpha>1$, there are no turning points and in addition to an incoming and outgoing wave for large positive x, there must also be an outgoing scattered wave

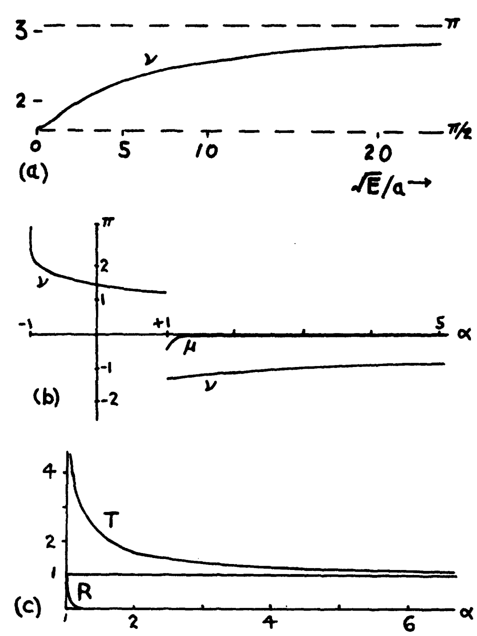

FIG. 3. $\nu(E)$ for $K^2(z)=E-2a/z$. (b) $\nu(E)$ and $\mu(E)$ for $K^2(z)=E+V_0\tanh(z/\beta)$. Note that μ is defined only for $\alpha=E/V_0\geq 1$, i.e., only for suprabarrier energies. (c) T and R for $K^2(z)=E+V_0\tanh(z/\beta)$. For $\alpha=E/V_0<1$, only R is defined and is identically 1.

for large negative x. It is convenient to set $\beta^2 V_0 = 1$, which is just a choice of the scale of z.

First, for $\alpha \leq 1$,

$$z_t = -\beta \tanh^{-1}\alpha, \quad -V_0 \leq E \leq V_0$$

$$S_{\rm CL}(x) = (a+1)^{1/2}\tanh^{-1}\left(\frac{\alpha + \tanh y}{\alpha+1}\right)^{1/2} - (1-\alpha)^{1/2}\tan^{-1}\left(\frac{\alpha+\tanh y}{1-\alpha}\right)^{1/2}$$

$$\underset{x\to+\infty}{\sim} z(E+V_0)^{1/2} + \phi,$$

$$S_{\rm NC}(x) = -(1-\alpha)^{1/2}\tanh^{-1}\left(\frac{\alpha+\tanh y}{\alpha-1}\right)^{1/2} + (1+\alpha)^{1/2}\tan^{-1}\left(\frac{\alpha+\tanh y}{-1-\alpha}\right)^{1/2}$$

$$\underset{x\to-\infty}{\sim} z(V_0-E)^{1/2} - \tfrac{1}{2}(1-\alpha)^{1/2}\ln[2(1-\alpha)] + (1+\alpha)^{1/2}\tan^{-1}\left(\frac{1-\alpha}{1+\alpha}\right)^{1/2}. \tag{23}$$

Here $y = z/\beta = z\sqrt{V_0}$ and

$$\phi = \tfrac{1}{2}(\alpha+1)^{1/2}\ln[2(1+\alpha)] - (1-\alpha)^{1/2}\tan^{-1}\left(\frac{1+\alpha}{1-\alpha}\right)^{1/2}. \tag{24}$$

Further,

$$(z')^{-1/2} = (S')^{-1/2}|E+V_0\tanh y|^{1/4} \underset{x\to\pm\infty}{\sim} (S')^{-1/2}|E\pm V_0|^{1/4} \approx 1,$$

$$v(z) = t^{(1-\alpha)^{1/2}/2}(1-t)^{-i(1+\alpha)^{1/2}/2}F(a,b,c;\,t), \tag{25}$$

where $t = \frac{1}{2}(1+\tanh y)$, $a = \frac{1}{2}(1-\alpha)^{1/2} - \frac{1}{2}i(1+\alpha)^{1/2}$, $b = 1+a$, $c = 1+(1-\alpha)^{1/2}$, and F is the hypergeometric function (AS, Chap. 15, Eqs. 15.3.6, particularly Sec. 15.5). The other linearly independent solution is discarded since it is irregular at $z=-\infty$ $(t=0)$.

Thus $\psi(x)\to 0$ exponentially for $x\to-\infty$, and

$$\Psi(x) \underset{x\to+\infty}{\sim} A\,e^{iS(x)-i\phi} + \text{c.c.},$$

where

$$A = \frac{\Gamma(1+(1-\alpha)^{1/2})\,\Gamma(i(1+\alpha)^{1/2})}{\Gamma(1+\frac{1}{2}(1-\alpha)^{1/2}+\frac{1}{2}i(1+\alpha)^{1/2})\,\Gamma(\frac{1}{2}(1-\alpha)^{1/2}+\frac{1}{2}i(1+\alpha)^{1/2})}. \tag{26}$$

Hence

$$R = 1, \qquad \nu = 2\phi - 2\arg A. \tag{27}$$

$\nu(E)$ is plotted in Fig. 3(b). Using various identities involving Γ functions (AS, p. 256), we write $\arg A$ as

$$\arg A = \arg\Gamma(1+i(1+\alpha)^{1/2}) - 2\arg\Gamma(\tfrac{1}{2}(1-\alpha)^{1/2}+\tfrac{1}{2}i(1+\alpha)^{1/2})\frac{\pi}{2} - \tan^{-1}\left(\frac{1+\alpha}{1-\alpha}\right)^{1/2}$$

$$= \sum_{n=0}^{\infty}\left[2\tan^{-1}\left(\frac{(1+\alpha)^{1/2}}{2n+(1-\alpha)^{1/2}}\right) - \tan^{-1}\left(\frac{(1+\alpha)^{1/2}}{n+1}\right)\right] - \tfrac{1}{2}\pi - \tan^{-1}\left(\frac{1+\alpha}{1-\alpha}\right)^{1/2}.$$

This form is handy for computation, since the two series cancel each other termwise almost exactly for even moderate n.

For $\alpha > 1$ there are no turning points. We arbitrarily (and conveniently) set $z_t = 0$. Then for all x (remember $y = z/\beta = z\sqrt{V_0}$)

$$S(x) = (\alpha+1)^{1/2}\left[\tanh^{-1}\left(\frac{\alpha+\tanh y}{\alpha+1}\right)^{1/2} - \tanh^{-1}\left(\frac{\alpha}{\alpha+1}\right)^{1/2}\right] - (\alpha-1)^{1/2}\left[\cosh^{-1}\left(\frac{\alpha+\tanh y}{\alpha-1}\right)^{1/2} - \coth^{-1}\left(\frac{\alpha}{\alpha-1}\right)^{1/2}\right]$$

$$\underset{x\to+\infty}{\sim} z(E+V_0)^{1/2} - \Theta_+$$

$$\underset{x\to-\infty}{\sim} z(E-V_0)^{1/2} + \Theta_-, \tag{28}$$

$$(z')^{-1/2} = (S')^{-1/2}|E+V_0\tanh y|^{1/4} \underset{x\to\pm\infty}{\sim} (S')^{-1/2}|E\pm V_0|^{1/4} \approx 1,$$

where

$$\Theta_+ = (\alpha+1)^{1/2}\left[\tanh^{-1}\left(\frac{\alpha}{\alpha+1}\right)^{1/2} - \tfrac{1}{2}\ln[2(1+\alpha)]\right] + (\alpha-1)^{1/2}\left[\tanh^{-1}\left(\frac{\alpha-1}{\alpha+1}\right)^{1/2} - \tanh^{-1}\left(\frac{\alpha-1}{\alpha}\right)^{1/2}\right],$$

$$\Theta_- = (\alpha+1)^{1/2}\left[\tanh^{-1}\left(\frac{\alpha-1}{\alpha+1}\right)^{1/2} - \tanh^{-1}\left(\frac{\alpha}{\alpha+1}\right)^{1/2}\right] + (\alpha-1)^{1/2}\left[\tanh^{-1}\left(\frac{\alpha-1}{\alpha}\right)^{1/2} - \tfrac{1}{2}\ln[2(\alpha-1)]\right], \tag{29}$$

and

$$v(z) = t^{(i/2)(\alpha-1)^{1/2}}(1-t)^{-(i/2)(\alpha+1)^{1/2}}t^{1-c}$$
$$\times F(a+1-c,\ b+1-c,\ 2-c;\ t). \qquad (30)$$

a, b, and c are as given immediately after (25). The $v(z)$ in (25) is still a solution, but one which is an *incoming* wave for large negative x instead of an outgoing wave.

Then, from (28)–(30),

$$\psi(x) \xrightarrow[x\to-\infty]{} e^{i\Theta_- - iS}$$
$$\xrightarrow[x\to+\infty]{} A\,e^{i(S+\Theta_+)} + Be^{-i(S+\Theta_+)},$$

where

$$A = \frac{\Gamma(1-i(\alpha-1)^{1/2})\,\Gamma(i(\alpha+1)^{1/2})}{\Gamma(1+\frac{1}{2}i[(\alpha+1)^{1/2}-(\alpha-1)^{1/2}])\,\Gamma(\frac{1}{2}i[(\alpha+1)^{1/2}-(\alpha-1)^{1/2}])},$$
$$B = \frac{\Gamma(1-i(\alpha-1))\,\Gamma(-i(\alpha+1)^{1/2})}{\Gamma(1-\frac{1}{2}i[(\alpha+1)^{1/2}+(\alpha-1)^{1/2}])\,\Gamma(-\frac{1}{2}i[(\alpha+1)^{1/2}+(\alpha-1)^{1/2}])}. \qquad (31)$$

Hence

$$T = \frac{1}{|B|^2} = \frac{\sinh[\pi(\alpha+1)^{1/2}]\sinh[\pi(\alpha-1)^{1/2}]}{\sinh^2\{\frac{1}{2}\pi[(\alpha+1)^{1/2}+(\alpha-1)^{1/2}]\}} \times\left(\frac{\alpha+1}{\alpha-1}\right)^{1/2},$$
$$R = \left|\frac{A}{B}\right|^2 = \frac{\sinh^2\{\frac{1}{2}\pi[(\alpha+1)^{1/2}-(\alpha-1)^{1/2}]\}}{\sinh^2\{\frac{1}{2}\pi[(\alpha+1)^{1/2}+(\alpha-1)^{1/2}]\}}, \qquad (32)$$

$$\mu = \Theta_+ + \Theta_- - \arg B,$$
$$\nu = -2\Theta_+ + \arg B - \arg A. \qquad (33)$$

For computational purposes we can write

$$\arg A = \sum_{n=1}^{\infty}\left[2\tan^{-1}\left(\frac{(\alpha+1)^{1/2}-(\alpha-1)^{1/2}}{2n}\right) - \tan^{-1}\left(\frac{(\alpha+1)^{1/2}}{n}\right) + \tan^{-1}\left(\frac{(\alpha-1)^{1/2}}{n}\right)\right],$$
$$\arg B = \sum_{n=1}^{\infty}\left[\tan^{-1}\left(\frac{(\alpha+1)^{1/2}}{n}\right) + \tan^{-1}\left(\frac{(\alpha-1)^{1/2}}{n}\right) - 2\tan^{-1}\left(\frac{(\alpha+1)^{1/2}+(\alpha-1)^{1/2}}{2n}\right)\right].$$

$\mu(E)$ and $\nu(E)$ are plotted in Fig. 3(b); $T(E)$ and $R(E)$ in Fig. 3(c).

Note that the equations $T+R=1$ and $\mu+\nu=\frac{1}{2}\pi$, which hold in general if $V(-\infty)=V(+\infty)$, do *not* hold here. [See the discussion following (38).]

III. TWO TURNING POINTS: BARRIERS

By two turning points we mean that for all energies E there are at most two values of x, called turning points and denoted by x_1 and x_2, with $x_1<x_2$, for which $k^2(x)=0$. In fact, for energy below the top of the barrier there are precisely two turning points; for energy above the top, none; and for energy at the top, one. Thus $V(x)$ is such that

$$V(x)\geqslant E,\quad x_1\leqslant x\leqslant x_2$$
$$\leqslant E,\quad x\leqslant x_1 \text{ or } x_2\leqslant x.$$

Hence between the turning points $k^2(x)$ is negative; we are in the nonclassical region. Outside the turning points, $k^2(x)$ is positive; we are in the classical region. The turning points in z are $z_i=z(x_i)$, $i=1,2$. K^2 is negative in the nonclassical region between z_1 and z_2 and positive in the classical region outside them (Fig. 4).

We define

$$S_+(x) = \int_{x_2}^{x} k\,dx = \int_{z_2}^{z} K\,dz \geqslant 0 \qquad (34)$$

in the classical region $x_2\leqslant x$,

$$S_-(x) = \int_{x_1}^{x} k\,dx = \int_{z_1}^{z} K\,dz \leqslant 0 \qquad (35)$$

in the classical region $x\leqslant x_1$, and

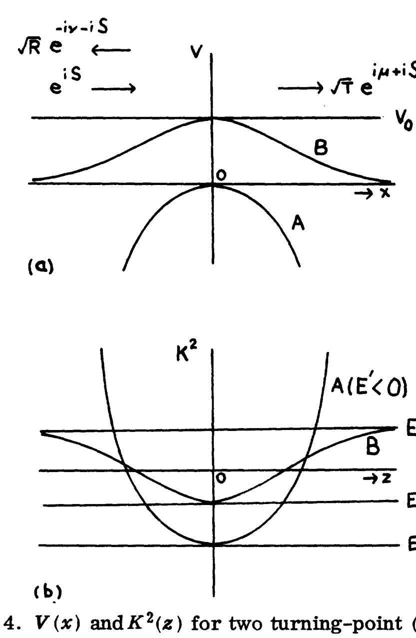

FIG. 4. $V(x)$ and $K^2(z)$ for two turning-point (barrier) problems. (a) $V(x)$ and the asymptotic forms for $\psi(x)$. (b) $K^2(z)$. (A) $K^2(z)=E+z^2/\beta^2$, (B) $K^2(z)=E-V_0\,\mathrm{sech}^2(z/\beta)$.

$$S_{NC}(x)=\int_{x_1}^{x}|k|\,dx=\int_{z_1}^{z}|K|\,dz\geqslant 0 \tag{36}$$

in the nonclassical region $x_1\leqslant x\leqslant x_2$. For all x,

$$S'(x)=\frac{d}{dx}S(x)=|k(x)|=z'|K(z)|\geqslant 0. \tag{37}$$

As customary, we seek a wave function ψ which has the asymptotic form of an incoming (from the left) wave of amplitude unity and a scattered wave:

$$e^{iS}+R^{1/2}e^{-i\nu}e^{-iS}\underset{x\to-\infty}{\sim}\psi(x)\underset{x\to+\infty}{\sim}T^{1/2}e^{i\mu}e^{iS}. \tag{38}$$

T and R are the transmission and reflection coefficients; μ and ν, the phase shifts of the transmitted and reflected waves. In general, $T+R=1$ and $\mu+\nu=\frac{1}{2}\pi$. This follows from properties of the Wronskian of the solutions of the Schrödinger equation.[13] The condition $T+R=1$ is conservation of flux and holds only if $k(-\infty)$ equals $k(+\infty)$, otherwise the condition is $R+[k(+\infty)/k(-\infty)]T=1$.

We will consider only two types of barrier here. The first [case (A)] is one for which $V(\pm\infty)=-\infty$; for the second [case (B)], $V(+\infty)=V(-\infty)<\infty$. For case (A)

(A) $V(\pm\infty)=-\infty,\quad -\infty\leqslant x\leqslant+\infty.$

We assume that the energy scale and x axis have been adjusted so that $V(0)=V_{\max}=0$. Thus $-\infty\leqslant E\leqslant+\infty$ and we choose

$$\text{(A)}\quad K^2(z)=E+z^2/\beta^2. \tag{39}$$

Thus $-\infty\leqslant z\leqslant\infty$, $K^2(\pm\infty)=k^2(\pm\infty)=+\infty$, and $z_1=-\beta\sqrt{-E}$, $z_2=+\beta\sqrt{-E}$. β is a positive constant of dimensions $(\text{length})^{+2}$. This is the Miller and Good approximation[2] in a slightly different form. For case (B),

(B) $V(+\infty)=V(-\infty)<\infty,\quad -\infty\leqslant x\leqslant+\infty.$

We adjust the energy scale and x axis so that $V(-\infty)=V(+\infty)=0$ and $V(0)=V_{\max}=V_0$. Thus $0\leqslant E$ and we choose

$$\text{(B)}\quad K^2(z)=E-V_0\,\text{sech}^2(z/\beta). \tag{40}$$

Thus $-\infty\leqslant z\leqslant\infty$, $K^2(\pm\infty)=k^2(\pm\infty)=E$ and $z_1=-\beta\,\text{sech}^{-1}(E/V_0)^{1/2}=-\beta\cosh^{-1}(V_0/E)^{1/2}$, $z_2=\beta\,\text{sech}^{-1}(E/V_0)^{1/2}=\beta\cosh^{-1}(V_0/E)^{1/2}$. β is a positive constant of dimension length.

In both (A) and (B) there is an as yet undetermined parameter β. It is determined, in terms of E and $V(x)$, by the requirement that

$$\int_{x_1}^{x_2}|k|\,dx\equiv W(E)=\int_{z_1}^{z_2}|K|\,dz \tag{41}$$

for E below the top of the barrier [$E\leqslant 0$ for (A) and $E\leqslant V_0$ for (B)] and

$$\left|\int_\Gamma k\,dx\right|\equiv W(E)=\left|\int_{\Gamma'}K\,dz\right| \tag{42}$$

for E above the top of the barrier. $\Gamma(\Gamma')$ is a straight-line contour between the complex zeros of $k(x)$ [$K(z)$] closest to the real axis.[14] Thus

$$\begin{aligned}&\text{(A)}\quad W(E)=\tfrac{1}{2}\pi\beta|E|,\\&\text{(B)}\quad W(E)=\pi\beta|\sqrt{V_0}-\sqrt{E}\,|.\end{aligned} \tag{43}$$

For case (A),

(A) $K^2(z)=E+z^2/\beta^2$,

and for $E\leqslant 0$,

$$\begin{aligned}&z_1=-\beta\sqrt{|E|},\quad z_2=+\beta\sqrt{|E|},\\&S_+=\frac{z}{2}\left(E+\frac{z^2}{\beta^2}\right)^{1/2}+\frac{\beta E}{2}\ln\left(\frac{z+(z^2+\beta^2E)^{1/2}}{(2\beta)^{1/2}}\right)\\&\qquad-\frac{\beta E}{4}\ln\left|\frac{\beta E}{2}\right|\underset{x\to+\infty}{\sim}\frac{z^2}{2\beta}+\frac{\beta E}{4}\ln\left|\frac{4ez^2}{\beta E}\right|,\\&S_-=\frac{z}{2}\left(E+\frac{z^2}{\beta^2}\right)^{1/2}-\frac{\beta E}{2}\ln\left(\frac{-z+(z^2+\beta^2E)^{1/2}}{(2\beta)^{1/2}}\right)\\&\qquad+\frac{\beta E}{4}\ln\left|\frac{\beta E}{2}\right|\underset{x\to-\infty}{\sim}\frac{-z^2}{2\beta}-\frac{\beta E}{4}\ln\left|\frac{4ez^2}{\beta E}\right|.\end{aligned} \tag{44}$$

The solutions to (2), $v''+(E+z^2/\beta^2)v=0$, are the parabolic cylinder functions $E(|\beta E/2|,\,z(2/\beta)^{1/2})$ and $E^*(|\beta E/2|,\,z(2/\beta)^{1/2})$ (AS, Chap. 19, Sec. 19.6–19.23). E has the proper asymptotic form, E^* does not; hence we discard E^*. Then

$$\begin{aligned}v(z)&\underset{x\to+\infty}{\sim}\left(\frac{2(2/\beta)^{1/2}}{z}\right)^{1/2}\\&\qquad\times\exp\left[i\left(\frac{z^2}{2\beta}+\frac{\beta E}{2}\ln z\left(\frac{2}{\beta}\right)^{1/2}+\frac{\phi}{2}+\frac{\pi}{4}\right)\right]\\&\underset{x\to+\infty}{\sim}\left(\frac{2(2/\beta)^{1/2}}{z}\right)^{1/2}\\&\qquad\times\exp\left[i\left(S_++\frac{\beta E}{4}\ln\left|\frac{\beta E}{2e}\right|+\frac{\phi}{2}+\frac{\pi}{4}\right)\right],\end{aligned} \tag{45}$$

where

$$\phi=\arg\Gamma(\tfrac{1}{2}-\tfrac{1}{2}i\beta E)=\arg\Gamma(\tfrac{1}{2}+iW/\pi). \tag{46}$$

Also

$$\begin{aligned}v(z)\underset{x\to-\infty}{\sim}i\left(\frac{2(2/\beta)^{1/2}}{|z|}\right)^{1/2}\Bigg\{&(1+e^{-\pi\beta E})^{1/2}\exp\left[-i\left(\frac{z^2}{2\beta}+\frac{\beta E}{2}\ln|z|\left(\frac{2}{\beta}\right)^{1/2}+\frac{\phi}{2}+\frac{\pi}{4}\right)\right]\\&-e^{-\pi\beta E/2}\exp\left[i\left(\frac{z^2}{2\beta}+\frac{\beta E}{2}\ln|z|\left(\frac{2}{\beta}\right)^{1/2}+\frac{\phi}{2}+\frac{\pi}{4}\right)\right]\Bigg\}\end{aligned}$$

$$\underset{x\to-\infty}{\sim} i\left(\frac{2(2/\beta)^{1/2}}{|z|}\right)^{1/2}\left\{(1+e^{-\pi\beta E})^{1/2}\exp\left[i\left(S_- - \frac{\beta E}{4}\ln\left|\frac{\beta E}{2e}\right| - \frac{\phi}{2} - \frac{\pi}{4}\right)\right]\right.$$
$$\left. - e^{-\pi\beta E/2}\exp\left[-i\left(S_- - \frac{\beta E}{4}\ln\left|\frac{\beta E}{2e}\right| - \frac{\phi}{2} - \frac{\pi}{4}\right)\right]\right\}. \qquad (47)$$

Hence, since $z'\to 1$ for $|x|$ large, we see from (38), (45), and (47) that

$$T=(1+e^{-\pi\beta E})^{-1}=(1+e^{2W})^{-1},$$
$$R=(1+e^{\pi\beta E})^{-1}=(1+e^{-2W})^{-1}; \qquad (48)$$

$$\mu=\frac{\beta E}{2}\ln\left|\frac{\beta E}{2e}\right|+\phi=\phi-\frac{W}{\pi}\ln\left|\frac{W}{\pi}\right|+\frac{W}{\pi},$$
$$\nu=\frac{\pi}{2}-\frac{\beta E}{2}\ln\left|\frac{\beta E}{2e}\right|-\phi=\frac{\pi}{2}-\phi+\frac{W}{\pi}\ln\left|\frac{W}{\pi}\right|-\frac{W}{\pi}. \qquad (49)$$

We have thus

$$T+R=1,$$
$$\mu+\nu=\tfrac{1}{2}\pi.$$

Note that T, R, μ, ν are given entirely in terms of $W=\int_{x_1}^{x_2}|k|\,dx$, i.e., entirely in terms of E and $V(x)$. The parameter β does not enter the solution at all except as a scaling factor for distance.

For $E\geq 0$, we pick $z_t=0$. Then (44)–(49) are correct for $E\geq 0$ also. The solution ψ is the same and so are all formulas for T, R, μ, ν (with W replaced by $-W$). These quantities are plotted as functions of W in Figs. 5 and 6.

For case (B),

(B) $K^2(z)=E-V_0\,\text{sech}^2(z/\beta)$.

We set $\alpha=(E/V_0)^{1/2}$. Then for $0\leq\alpha\leq+1$,

$$z_1=-\beta\,\text{sech}^{-1}\alpha,\quad z_2=+\beta\,\text{sech}^{-1}\alpha. \qquad (50)$$

Thus

$$S_\pm=\beta(E)^{1/2}\tanh^{-1}t-\beta(V_0)^{1/2}\tanh^{-1}(\alpha t)$$
$$\underset{\pm\infty}{\sim} z\sqrt{E}\mp\phi, \qquad (51)$$

where

$$t=\left(\frac{\alpha^2-\text{sech}^2(z/\beta)}{\alpha^2\tanh^2(z/\beta)}\right)^{1/2}, \qquad (52)$$

$$\phi=\tfrac{1}{2}\beta(E)^{1/2}\ln\left(\frac{1-\alpha^2}{\alpha^2}\right)+\beta(V_0)^{1/2}\tanh^{-1}\alpha, \qquad (53)$$

and $S_+(S_-)$ takes the positive (negative) branch of the square root defining t.

The solutions of (2) are hypergeometric functions (AS, Chap. 15):

$$v_1=[\text{sech}(z/\beta)]^{2i\gamma}F(a,b,\tfrac{1}{2};\tanh^2(z/\beta)),\quad\text{even}$$
$$v_2=\tanh(z/\beta)[\text{sech}(z/\beta)]^{2i\gamma}\times F(c-a,c-b,\tfrac{3}{2};\tanh^2(z/\beta)),\quad\text{odd} \qquad (54)$$

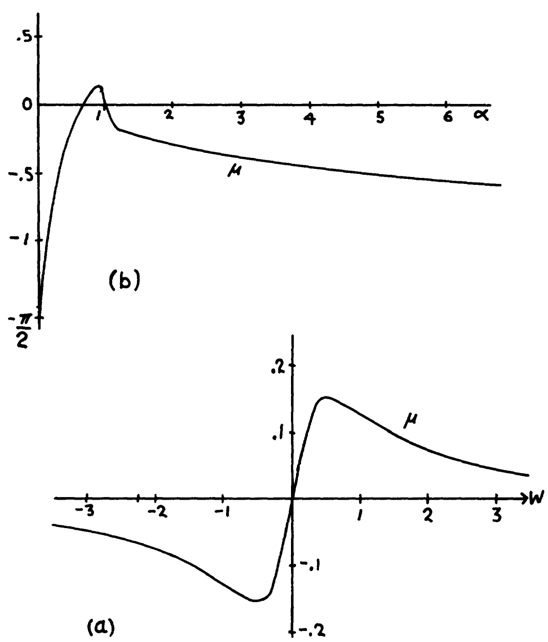

FIG. 5. Transmitted phase shift $\mu(E)$. (a) $K^2(z)=E+z^2/\beta^2$. Here $W=\frac{1}{2}\pi\beta E$. (b) $K^2(z)=E-V_0\,\text{sech}^2(z/\beta)$. Here $\alpha=(E/V_0)^{1/2}$. Note that in both cases $\mu(0)=0$ and $\mu+\nu=\frac{1}{2}\pi$.

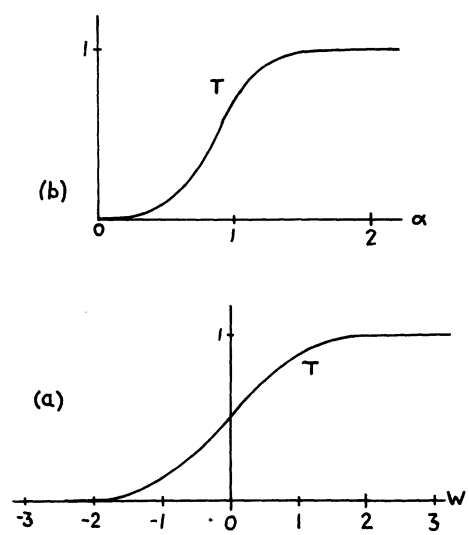

FIG. 6. Transmission coefficient $T(E)$. (a) $K^2(z)=E+z^2/\beta^2$. Again $W=\frac{1}{2}\pi\beta E$. (b) $K^2(z)=E-V_0\,\text{sech}^2(z/\beta)$. Again $\alpha=(E/V_0)^{1/2}$. In both cases the reflection coefficient is given by $R=1-T$.

where

$$\gamma = \tfrac{1}{2} i\beta\sqrt{E}$$
$$a = \gamma + \tfrac{1}{4} + \tfrac{1}{4}(1 - 4\beta^2 V_0)^{1/2},$$
$$b = \gamma + \tfrac{1}{4} - \tfrac{1}{4}(1 - 4\beta^2 V_0)^{1/2}, \qquad (55)$$
$$c = 2\gamma + 1.$$

Since $z' \to 1$ for $|x| \to \infty$, using AS, Eq. 15.3.6, we have

$$\psi_1(x) \underset{x\to\pm\infty}{\sim} A[\cosh(z/\beta)]^{-i\beta\sqrt{E}} + \text{c.c.},$$
$$\psi_2(x) \underset{x\to\pm\infty}{\sim} \pm B[\cosh(z/\beta)]^{-i\beta\sqrt{E}} + \text{c.c.}, \qquad (56)$$

where c.c. stands for complex conjugate and

$$A = \frac{\Gamma(\frac{1}{2})\Gamma(-i\beta\sqrt{E})}{\Gamma(\frac{1}{4} - \frac{1}{2}i\beta\sqrt{E} - \frac{1}{4}(1-4\beta^2V_0)^{1/2})\Gamma(\frac{1}{4} - \frac{1}{2}i\beta\sqrt{E} + \frac{1}{4}(1-4\beta^2V_0)^{1/2})},$$
$$B = \frac{\Gamma(\frac{1}{2})\Gamma(-i\beta\sqrt{E})}{\Gamma(\frac{3}{4} - \frac{1}{2}i\beta\sqrt{E} + \frac{1}{4}(1-4\beta^2V_0)^{1/2})\Gamma(\frac{3}{4} - \frac{1}{2}i\beta\sqrt{E} - \frac{1}{4}(1-4\beta^2V_0)^{1/2})}. \qquad (57)$$

Hence, using $\cosh(z/\beta) \to \frac{1}{2}e^{\pm z/\beta}$ as $|x| \to \infty$, we have

$$\psi_1(x) \underset{\pm\infty}{\sim} A\, 2^{i\beta\sqrt{E}} e^{\mp iz\sqrt{E}} + \text{c.c.}$$
$$\underset{\pm\infty}{\sim} A\, 2^{i\beta\sqrt{E}} e^{\mp i(S_\pm \pm\phi)} + \text{c.c.},$$
$$\psi_2(x) \underset{\pm\infty}{\sim} \pm(B\, 2^{i\beta\sqrt{E}} e^{\mp iz\sqrt{E}} + \text{c.c.}) \qquad (58)$$
$$\underset{\pm\infty}{\sim} \pm(B\, 2^{i\beta\sqrt{E}} e^{\mp i(S_\pm \pm\phi)} + \text{c.c.}).$$

Taking the linear combination $a\psi_1 + b\psi_2 = \psi$ such that

$$e^{iS} + R^{1/2}e^{-i\nu}e^{-iS} \underset{-\infty}{\sim} \psi \underset{+\infty}{\sim} T^{1/2}e^{i\mu}e^{iS},$$

we find that

$$a = 2^{-1-i\beta\sqrt{E}}(1/A)e^{i\phi},$$
$$b = -aA/B.$$

Thus

$$T^{1/2}e^{i\mu} = \frac{1}{2}\left(\frac{A^*}{A} - \frac{B^*}{B}\right)e^{2i\phi - i2\beta E^{1/2}\ln 2},$$
$$R^{1/2}e^{-i\nu} = \frac{1}{2}\left(\frac{A^*}{A} + \frac{B^*}{B}\right)e^{2i\phi - i2\beta E^{1/2}\ln 2}, \qquad (59)$$

and, using the Γ-function formulas (AS, p.256),

$$T = \frac{1}{4}\left|\frac{A^*}{A} - \frac{B^*}{B}\right|^2 = \left(1 + \frac{\cosh^2[\pi(\beta^2V_0 - \frac{1}{4})^{1/2}]}{\sinh^2(\pi\beta\sqrt{E})}\right)^{-1},$$
$$R = \frac{1}{4}\left|\frac{A^*}{A} + \frac{B^*}{B}\right|^2 = \left(1 + \frac{\sinh^2(\pi\beta\sqrt{E})}{\cosh^2[\pi(\beta^2V_0 - \frac{1}{4})^{1/2}]}\right)^{-1}; \qquad (60)$$

$$\mu = \tfrac{1}{2}\pi + 2\phi + 2\arg\Gamma(i\beta\sqrt{E}) - \arg\Gamma(\tfrac{1}{2} + i[\beta\sqrt{E} + (\beta^2V_0 - \tfrac{1}{4})^{1/2}]) - \arg\Gamma(\tfrac{1}{2} + i[\beta\sqrt{E} - (\beta^2V_0 - \tfrac{1}{4})^{1/2}]),$$

$$\nu = \tfrac{1}{2}\pi - \mu. \qquad (61)$$

For $\alpha^2 > 1$, we set $z_t = 0$. Then (51) still holds if we replace ϕ by

$$\phi = \tfrac{1}{2}\beta E^{1/2}\ln\left|\frac{\alpha^2-1}{\alpha^2}\right| + \tfrac{1}{2}\beta V_0^{1/2}\ln\left|\frac{1+\alpha}{1-\alpha}\right|. \qquad (62)$$

For $\alpha^2 < 1$, this of course is the same as (53). Then all the other formulas (51)–(61) hold, and T, R, μ, ν are given still by (60) and (61), with (62) for ϕ. T, R, μ, and ν are plotted in Figs. 5 and 6.

We see that here the parameter β is still evident in the final formulas. β appears really only as a scaling factor for z. It is convenient to set $\beta^2V_0 = 1$ (this choice has the proper dimensions). Then $(\beta^2V_0 - \frac{1}{4})^{1/2}$ is replaced by $(\frac{3}{4})^{1/2}$ and $\beta\sqrt{E}$ by $\alpha = (E/V_0)^{1/2}$. Thus

$$T = \left(1 + \frac{\cosh^2(\frac{1}{2}\pi\sqrt{3})}{\sinh^2(\pi\alpha)}\right)^{-1},$$
$$R = \left(1 + \frac{\sinh^2(\pi\alpha)}{\cosh^2(\frac{1}{2}\pi\sqrt{3})}\right)^{-1}; \qquad (60')$$

$$\mu = \tfrac{1}{2}\pi + 2\phi + 2\arg\Gamma(i\alpha) - \arg\Gamma(\tfrac{1}{2} + i(\alpha + \tfrac{1}{2}\sqrt{3})) - \arg\Gamma(\tfrac{1}{2} + i(\alpha - \tfrac{1}{2}\sqrt{3})),$$
$$\nu = \tfrac{1}{2}\pi - \mu; \qquad (61')$$

where

$$\phi = \tfrac{1}{2}\alpha\ln\left|\frac{\alpha^2-1}{\alpha^2}\right| + \tfrac{1}{2}\ln\left|\frac{1+\alpha}{1-\alpha}\right|. \qquad (62')$$

This choice of $\beta^2V_0 = 1$ has been made in Fig. 5.

IV. TWO TURNING POINTS: WELLS

The situation here is precisely the opposite of that for potential barriers. Here $k^2(x)$ and $K^2(z)$ are positive in the classical region *between* the turning points x_1 and x_2 (z_1 and z_2) and negative in the nonclassical regions *outside* the turning points (Fig. 7). Except in one case, we consider the bound-state spectrum only.

We consider the following types of potentials.

For case (A), $-\infty \leq x \leq \infty$, $V(\pm\infty) = +\infty$. We assume that the energy scale and x axis have been adjusted so that $V(0) = V_{\min} = 0$. Thus $E \geq 0$ and we

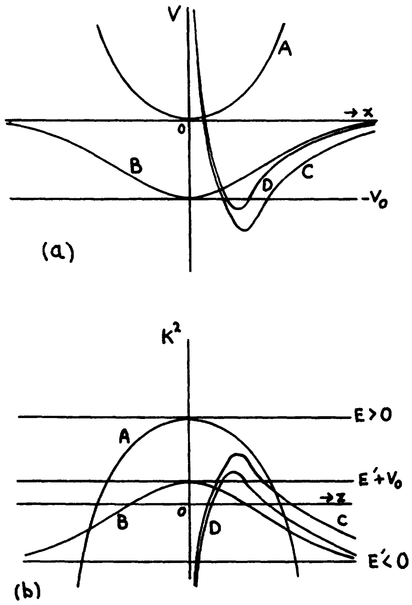

FIG. 7. $V(x)$ and $K^2(z)$ for two-turning point (well) problems. (a) $V(x)$. (b) $K^2(z)$. (A) $K^2(z)=E-z^2/\beta^2$. (B) $K^2(z)=E+V_0\,\mathrm{sech}^2(z/\beta)$. (C) $K^2(z)=E+e^2/z-l(l+1)/z^2$. (D) $K^2(z)=E+\lambda\exp(-z/\beta)[1-\exp(-z/\beta)]^{-1}-b\exp(-z/\beta)[1-\exp(-z/\beta)]^{-2}$.

choose

$$\text{(A)}\quad K^2(z)=E-z^2/\beta^2. \tag{63}$$

Thus $-\infty\leq z\leq+\infty$, $K^2(\pm\infty)=-\infty$, and $z_1=-\beta\sqrt{E}$, $z_2=+\beta\sqrt{E}$. β is a positive constant of dimension (length)$^{+2}$. This is again the Miller and Good approximation.[2]

For case (B), $-\infty\leq x\leq\infty$, $|V_{\min}|<V(+\infty)=V(-\infty)<\infty$. We adjust the energy scale and x axis so that $V(\pm\infty)=0$ and $V(0)=V_{\min}\equiv-V_0$. Then $E\geq-V_0$ and we choose

$$\text{(B)}\quad K^2(z)=E+V_0\,\mathrm{sech}^2(z/\beta). \tag{64}$$

Thus $-\infty\leq z\leq\infty$, $K^2(\pm\infty)=k^2(\pm\infty)=E$, $K^2(0)=k^2(0)=E+V_0$, and $z_1=-\beta\,\mathrm{sech}^{-1}(|E|/V_0)$, $z_2=\beta\,\mathrm{sech}^{-1}(|E|/V_0)$ for $E\leq0$; for $E>0$ there are no turning points.

For case (C), $0\leq x\leq\infty$, $V(x)\sim+x^{-2}$ as $x\to0$, $V(x)\sim-x^{-1}$ as $x\to\infty$ and $V(x)$ has a minimum for some positive x. Thus, $V(x)$ is supposed to have the long-range behavior of the Coulomb potential and the short-range behavior of the centrifugal x^{-2} barrier. We again assume that $V(\infty)=0$ and hence choose precisely the radial effective attractive Coulomb potential:

$$\text{(C)}\quad K^2(z)=E+e^2/z-l(l+1)/z^2. \tag{65}$$

Thus $0\leq z\leq\infty$, $K^2(0)\sim z^{-2}$, $K^2(\infty)=E$, and $z_1=(-e^2/2E)-[(e^2/2E)^2-l(l+1)/E]^{1/2}$, $z_2=(-e^2/2E)+[(e^2/2E)^2-l(l+1)/E]^{1/2}$ for $E<0$. For $E>0$ there is only one turning point; we will not discuss this situation.

For case (D), $0\leq x\leq\infty$, $V(x)\sim+x^{-2}$ as $x\to0$, $V(x)$ has a minimum at some positive x, but $V(x)$ goes to zero more rapidly at plus infinity than the Coulomb potential. In fact, we shall choose a $K^2(z)$ which goes exponentially rapidly to zero. Again, we assume $V(\infty)=0$ and choose a variant of the Eckart potential,[19,21]

$$\text{(D)}\quad K^2(z)=E+\frac{\lambda e^{-z/\beta}}{1-e^{-z/\beta}}-\frac{be^{-z/\beta}}{(1-e^{-z/\beta})^2}. \tag{66}$$

λ and b are positive constants of dimension (length)$^{-2}$, $\lambda>b$ [this ensures that $K^2(z)$ has a local maximum for $x>0$], and β is a positive constant of dimension (length)$^{+1}$. Thus $0\leq z\leq\infty$, $K^2(\infty)=k^2(\infty)=E$, and

$$z_1=-\beta\ln\left(\frac{\lambda-b-2E+[(\lambda-b)^2+4Eb]^{1/2}}{2(\lambda-E)}\right),$$

$$z_2=-\beta\ln\left(\frac{\lambda-b-2E-[(\lambda-b)^2+4Eb]^{1/2}}{2(\lambda-E)}\right)$$

for $E<0$. If $E>0$, there is only one turning point; we again will not discuss this situation.

The essential difference between (A) and (B) and between (C) and (D) is that (A) and (C) have an infinite number of bound states, while (B) and (D) have a finite number of bound states. For (C) and (D), it is known that for attractive potentials which behave at the origin like the centrifugal barrier, x^{-2}, then the energy spectrum for $E\leq0$ consists of a finite number of discrete levels if $V(x)$ falls off at least as fast as x^{-4} for large x and an infinite number of discrete states (bounded from below) if it falls off slower.[15,16] We illustrate this with x^{-1} (C) and $e^{-x/\beta}$ (D).

The boundary conditions we put on $\psi(x)$ are $\psi(\pm\infty)=0$ for types (A) and (B) and $\psi(0)=\psi(+\infty)=0$ for types (C) and (D) for negative energies.

Just as for potential barriers we fixed the "extra" parameters in $K^2(z)$ in terms of E and $V(x)$ by integrating $k(x)$ and $K(z)$ between their turning points, we here must demand

$$\Phi(E;V)=\int_{x_1}^{x_2}k\,dx=\int_{z_1}^{z_2}K\,dt. \tag{67}$$

Φ is the integral over the classical region (for *two* turning points) and is hence the classical action of the well, divided by $2\hbar$. We therefore expect quantization conditions similar to the Bohr-Sommerfeld rule $\Phi=(n+\frac{1}{2})\pi$.

The precise definitions of the quantity $S(x)$ differs somewhat from type to type here; so they will be given in each case separately.

For case (A),

$$\text{(A)}\quad K^2(z)=E-z^2/\beta^2.$$

Here we have two turning points for all $E>0$; so we define

$$S_+ = \int_{x_2}^{x} |k|\,dx = \int_{z_2}^{z} |K|\,dz$$
$$= \frac{z}{2}\left(\frac{z^2}{\beta^2} - E\right)^{1/2} - \frac{\beta E}{2}\ln\left(\frac{z + (z^2 - \beta^2 E)^{1/2}}{\beta\sqrt{E}}\right),$$
$$S_- = \int_{x_1}^{x} |k|\,dx = \int_{z_1}^{z} |K|\,dz$$
$$= \frac{z}{2}\left(\frac{z^2}{\beta^2} - E\right)^{1/2} + \frac{\beta E}{2}\ln\left(\frac{-z + (z^2 - \beta^2 E)^{1/2}}{\beta\sqrt{E}}\right) \tag{68}$$

for $x > x_2$ and $x < x_1$, respectively. Also, for all x,

$$(z')^{-1/2} = (S')^{-1/2}|z^2/\beta^2 - E|^{1/4} \underset{x\to\pm\infty}{\sim} (S')^{-1/2}(|z|/\beta)^{1/2}, \tag{69}$$

and

$$S_\pm(x) \underset{x\to\pm\infty}{\sim} \pm\frac{z^2}{2\beta} \mp \frac{\beta E}{2}\ln\left(\frac{2|z|}{\beta\sqrt{E}}\right) \mp \frac{\beta E}{4}. \tag{70}$$

The dimensionless action Φ is given by

$$\Phi(E) = \int_{x_1}^{x_2} k\,dx = \int_{z_1}^{z_2} K\,dz$$
$$= \int_{-\beta\sqrt{E}}^{+\beta\sqrt{E}} (E - z^2/\beta^2)^{1/2}\,dz = \tfrac{1}{2}\pi\beta E. \tag{71}$$

The solutions to $v''(z) + (E - z^2/\beta^2)v = 0$ are the parabolic cylinder functions (AS, Sec. 19.2–19.10) $U(-\frac{1}{2}\beta E,\ z(2/\beta)^{1/2})$ and $V(-\frac{1}{2}\beta E,\ z(2/\beta)^{1/2})$. Of these, V is singular at $\pm\infty$; so the solutions are

$$\psi(x) = (z')^{-1/2}U(-\tfrac{1}{2}\beta E,\ z(2/\beta)^{1/2}). \tag{72}$$

We have

$$\psi(x) \underset{x\to+\infty}{\sim} (S')^{-1/2}\left(\frac{|z|}{2}\right)^{1/2} \frac{\Gamma(\frac{1}{2}+\frac{1}{2}\beta E)^{1/2}\exp[-\frac{1}{2}z(z^2/\beta^2 - E)^{1/2}] + \frac{1}{2}\beta E\ln[z(2/\beta)^{1/2}]}{(2\pi)^{1/4}(2z^2/\beta - 2\beta E)^{1/2}}$$
$$\underset{x\to+\infty}{\sim} (S')^{-1/2}(\tfrac{1}{4}|z|\beta)^{1/2}(2\pi)^{-1/4}(z^2 - \beta^2 E)^{-1/2}[\Gamma(\tfrac{1}{2} - \tfrac{1}{2}\beta E)]^{1/2}\exp[-S_+ + \tfrac{1}{4}\beta E\ln(\tfrac{1}{4}\beta E)]$$
$$\underset{x\to+\infty}{\longrightarrow} 0, \tag{73}$$

$$\psi(x) \underset{x\to-\infty}{\sim} (S')^{-1/2}(\tfrac{1}{4}|z|\beta)^{1/2}(z^2 - \beta^2 E)^{-1/2}[\Gamma(\tfrac{1}{2} + \tfrac{1}{2}\beta E)]^{1/2}(2\pi)^{-1/4}$$
$$\times\left[\sin\frac{\pi\beta E}{2}\exp\left(-S - \frac{\beta E}{4}\ln\frac{\beta E}{4}\right) + \frac{\exp[S_- + \frac{1}{4}\beta E\ln(\frac{1}{4}\beta E)]}{\Gamma(\frac{1}{2}(1+\beta E))\,\Gamma(\frac{1}{2}(1-\beta E))}\right]. \tag{74}$$

Now, the last term in (74) blows up at minus infinity unless its coefficient is zero, i.e., unless

$$\frac{1}{\Gamma(\frac{1}{2} - \frac{1}{2}\beta E)} = 0;$$

hence $\frac{1}{2} - \frac{1}{2}\beta E = -n$, $n+0, 1, 2, \ldots$. The quantization condition is thus

$$\Phi(E) = \tfrac{1}{2}\beta\pi E = (n + \tfrac{1}{2})\pi, \tag{75}$$

precisely the Bohr-Sommerfeld rule, and for $\frac{1}{2}\beta E$ a half-integer, U is just a Hermite polynomial; so

$$\psi(x) = (S')^{-1/2}|E - z^2/\beta^2|^{1/4}\,2^{-n/2}e^{-z^2/2\beta}H_n(z/\sqrt{\beta}). \tag{76}$$

For case (B),

(B) $K^2(z) = E + V_0\,\mathrm{sech}^2(z/\beta)$.

We discuss $E \le 0$ and $E \ge 0$ separately. First, for $E \le 0$, there are two turning points, and similarly to (A), we have ($\alpha = E/V_0$)

$$S_\pm(x) = \beta|E|^{1/2}\tanh^{-1}|t| \mp \beta V_0^{1/2}\tanh^{-1}(|t|\,|\alpha|^{1/2}) \underset{x\to\pm\infty}{\sim} z\sqrt{E} \tag{77}$$

and for all x

$$(z')^{-1/2} = (S')^{-1/2}[E + V_0\,\mathrm{sech}^2(z/\beta)]^{1/4} \underset{x\to\pm\infty}{\longrightarrow} 1. \tag{78}$$

Φ is given by

$$\Phi(E,\ V_0,\ \beta) = \int_{z_1}^{z_2}[E + V_0\,\mathrm{sech}^2(z/\beta)]^{1/2}\,dz$$
$$= \beta\pi(\sqrt{V_0} - \sqrt{|E|}). \tag{79}$$

The solutions to $v'' + [E + V_0\,\mathrm{sech}^2(z/\beta)]v = 0$ are

$$v_1(z) = [\cosh(z/\beta)]^{-2\sigma}F(a,\ b,\ \tfrac{1}{2};\ \tanh^2(z/\beta)), \text{ even}$$

and

$$v_2(z) = \tanh(z/\beta)[\cosh(z/\beta)]^{-2\sigma} \times F(c-a,\ c-b,\ \tfrac{3}{2};\ \tanh^2(z/\beta)), \text{ odd} \tag{80}$$

where

$$\sigma = \tfrac{1}{2}\beta\sqrt{|E|},$$
$$a = \sigma + \tfrac{1}{4} + \tfrac{1}{4}(1 + 4\beta^2 V_0)^{1/2},$$
$$b = \sigma + \tfrac{1}{4} - \tfrac{1}{4}(1 + 4\beta^2 V_0)^{1/2}, \tag{81}$$
$$c = 2\sigma + 1.$$

$F(a, b, c; x)$ is the hypergeometric function (AS, Chap. 15). For large x,

$$v_1 \underset{x\to\pm\infty}{\sim} A[\cosh(z/\beta)]^{-2\sigma} + B[\cosh(z/\beta)]^{2\sigma}$$

$$\underset{x\to\pm\infty}{\sim} A\,2^{2\sigma} e^{\mp x\sqrt{|E|}} + B\,2^{-2\sigma} e^{\pm x\sqrt{|E|}}$$

and (82)

$$v_2 \underset{x\to\pm\infty}{\sim} \pm C[\cosh(z/\beta)]^{-2\sigma} \pm D[\cosh(z/\beta)]^{+2\sigma}$$

$$\underset{x\to\pm\infty}{\sim} \pm C\,2^{2\sigma} e^{\mp x\sqrt{|E|}} \pm D\,2^{-2\sigma} e^{\pm x\sqrt{|E|}},$$

where

$$A = \frac{\Gamma(\tfrac{1}{2})\Gamma(\tfrac{1}{2}-a-b)}{\Gamma(\tfrac{1}{2}-a)\Gamma(\tfrac{1}{2}-b)},$$

$$B = \frac{\Gamma(\tfrac{1}{2})\Gamma(a+b-\tfrac{1}{2})}{\Gamma(a)\Gamma(b)}, \qquad (83)$$

$$C = \frac{\Gamma(\tfrac{3}{2})\Gamma(\tfrac{3}{2}-2c+a+b)}{\Gamma(\tfrac{3}{2}+b-c)\Gamma(\tfrac{3}{2}+a-c)},$$

$$D = \frac{\Gamma(\tfrac{3}{2})\Gamma(2c-\tfrac{3}{2}-a-b)}{\Gamma(c-b)\Gamma(c-a)}.$$

Hence v_1 remains finite at $\pm\infty$ only if $B=0$, hence only if a or b is a negative integer. Since a is positive, we have that

$$b = \tfrac{1}{2}\beta\sqrt{|E|} + \tfrac{1}{4} - \tfrac{1}{4}(1+4\beta^2 V_0)^{1/2} = -n, \quad n = 0, 1, 2, \ldots$$

$$\Phi = \beta\pi(\sqrt{V_0} - \sqrt{|E|}) = \beta\pi\sqrt{V_0} - 2\pi\sigma = (2n+\rho)\pi, \qquad (84)$$

where

$$\rho = \tfrac{1}{2} + \beta\sqrt{V_0} - \tfrac{1}{2}(1+4\beta^2 V_0)^{1/2}.$$

Similarly, v_2 remains finite only if $D=0$; hence

$$\Phi = (2n+1+\rho)\pi. \qquad (85)$$

Hence, in general,

$$\Phi = (m+\rho)\pi,$$

and the parity of $\psi(x)$ is $(-1)^m$.

There are a finite number of bound states, since $\sigma > 0$ implies

$$m \le \tfrac{1}{2}(1+4\beta^2 V_0)^{1/2} - \tfrac{1}{2}.$$

If we set $\beta^2 V_0 = l(l+1)$, this is

$$m \le l;$$

so

$$\Phi = (m+\rho)\pi, \quad m = 0, 1, \ldots, l. \qquad (86)$$

$$\rho = [l(l+1)]^{1/2} - l.$$

For $E > 0$, we choose $z_t = 0$; hence

$$S_\pm = \int_0^x K\,dz = \beta E^{1/2}\sinh^{-1}\left[\left(\frac{E}{E+V_0}\right)^{1/2}\sinh\frac{z}{\beta}\right]$$

$$+\beta V_0^{1/2}\sin^{-1}\left[\left(\frac{V_0}{E+V_0}\right)^{1/2}\tanh\frac{z}{\beta}\right]$$

$$\underset{x\to\pm\infty}{\sim} z\sqrt{E} \pm \phi$$

where

$$\phi = \beta E^{1/2}\ln\left(\frac{E}{E+V_0}\right) + \beta V_0^{1/2}\sin^{-1}\left(\frac{V_0}{E+V_0}\right). \qquad (87)$$

Then the same solutions hold for $E > 0$ as for $E < 0$, with $\sigma = \tfrac{1}{2}\beta\sqrt{|E|}$ replaced by $\sigma = \tfrac{1}{2}i\beta\sqrt{E}$. Thus

$$\psi_1(x) \underset{x\to\pm\infty}{\sim} A\,2^{i\beta\sqrt{E}} e^{\mp iS_\pm + i\phi} + \text{c.c.},$$

$$\psi_2(x) \underset{x\to\pm\infty}{\sim} C\,2^{i\beta\sqrt{E}} e^{\mp iS_\pm + i\phi} + \text{c.c.} \qquad (88)$$

We take the linear combination of these two which has the asymptotic properties

$$e^{iS_-} + R^{1/2} e^{-i\nu} e^{-iS_-} \underset{x\to-\infty}{\sim} \psi \underset{x\to+\infty}{\sim} T^{1/2} e^{i\mu} e^{iS_+},$$

obtaining

$$\mu = \tfrac{1}{2}\pi - \nu$$

$$= \tfrac{1}{2}\pi - 2\phi + \tan^{-1}\{\tan[\tfrac{1}{2}\pi(1+4\beta^2 V_0)^{1/2}]\tanh(\pi\sqrt{E})\}$$

$$+ 2\arg[\Gamma(i\beta\sqrt{E})\Gamma(\tfrac{1}{2}+\tfrac{1}{2}(1+4\beta^2 V_0)^{1/2} - i\beta\sqrt{E})],$$

$$T = \frac{1}{4}\left|\frac{A}{A^*} - \frac{C}{C^*}\right|^2 = \left(1 + \frac{\cos^2(\tfrac{1}{2}\pi(1+4\beta^2 V_0)^{1/2})}{\sinh^2(\pi\beta\sqrt{E})}\right)^{-1},$$

$$R = 1 - T = \frac{1}{4}\left|\frac{A}{A^*} + \frac{C}{C^*}\right|^2$$

$$= \left(1 + \frac{\sinh^2(\pi\beta\sqrt{E})}{\cos^2(\tfrac{1}{2}\pi(1+4\beta^2 V_0)^{1/2})}\right)^{-1}. \qquad (89)$$

T and μ are plotted in Fig. 8 as functions of E.

Note that as a function of $\beta^2 V_0$, $T(R)$ has a maxi-

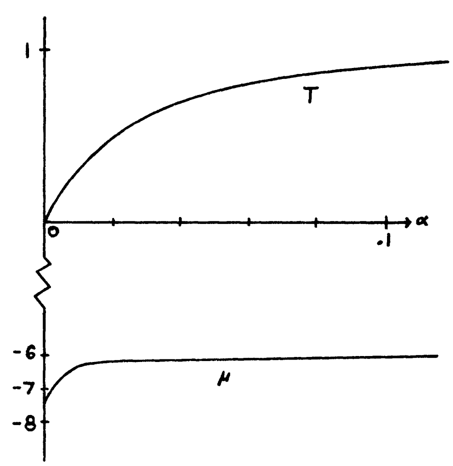

FIG. 8. Transmission coefficient T and transmitted phase shift μ for suprawell energies for $K^2(x) = E - V_0 \times \text{sech}^2(z/\beta)$, $\alpha = E/V_0 \ge 0$. We have taken $\beta^2 V_0 = \frac{15}{4}$. The transmission coefficient R is given by $R = 1 - T$ and the reflected phase shift $\mu = \frac{1}{2}\pi - \nu$.

mum (minimum) for $\beta^2 V_0 = l(l+1)$, l any integer. Thus, for those wells such that $\Phi(E=0, \beta^2 V_0 = l(l+1)) = \pi[l(l+1)]^{1/2} = \pi\beta\sqrt{V_0}$, we find $T=1$ and $R=0$, i.e., no reflection occurs. In this case, $\mu = \frac{1}{2}\pi - 2\phi \to \frac{1}{2}\pi$ as $E\to\infty$. Also T exhibits a minimum for $\beta^2 V_0 = (l+\frac{1}{2})(l-\frac{1}{2})$: $T(E) = \tanh^2(\pi\beta\sqrt{E})$, $R = \text{sech}^2(\pi\beta\sqrt{E})$. That is, $T(R)$ has a minimum (maximum) for wells such that $\Phi(E=0, \beta^2 V_0 = l^2 - \frac{1}{4}) = \pi(l^2-\frac{1}{4})^{1/2}$.

For case (C),

$$\text{(C)}\ K^2(z) = E + e^2/z - l(l+1)/z^2.$$

For $E<0$, there are two turning points. We have

$$S_+ = \int_{z_2}^{z} |K|\,dz = \sqrt{X} - \frac{e^2}{2\sqrt{|E|}} \ln\left(\frac{e^2/2E + z + (-X/E)^{1/2}}{[e^4/4E^2 - l(l+1)/E]^{1/2}}\right) - [l(l+1)]^{1/2} \ln\left(\frac{2l(l+1) - e^2 z + 2[l(l+1)X]^{1/2}}{2l(l+1) - e^2 z_2}\ \frac{z_2}{z}\right)$$

$$\underset{x\to+\infty}{\sim} z\sqrt{|E|},$$

where

$$X = -Ez^2 - e^2 z + l(l+1),$$

$$S_- = \int_{z_1}^{z} |K|\,dx = \sqrt{X} - \frac{e^2}{2\sqrt{|E|}} \ln\left(\frac{-e^2/2E - z - (-X/E)^{1/2}}{[e^4/2E^2 - l(l+1)/E]^{1/2}}\right) - [l(l+1)]^{1/2} \ln\left(\frac{2l(l+1) - e^2 z + 2[l(l+1)X]^{1/2}}{2l(l+1) - e^2 z_1}\ \frac{z_1}{z}\right)$$

$$\underset{x\to0}{\sim} [l(l+1)]^{1/2} \ln z,$$

$$(z')^{-1/2} = (S')^{-1/2} |K(z)|^{1/2} \underset{x\to+\infty}{\sim} 1 \underset{x\to0}{\sim} (S')^{-1/2} |l(l+1)/z^2|^{1/4},$$

and

$$\Phi = \int_{z_1}^{z_2} |K|\,dz = \int_{z_1}^{z_2} [Ez^2 + e^2 z - l(l+1)]^{1/2} dz = \pi\{e^2/2\sqrt{|E|} - [l(l+1)]^{1/2}\}. \quad (90)$$

The solutions to $v'' + K^2(z)v = 0$ which are regular at the origin are[17] (AS, Eq. 22.6.17)

$$v(z) = (2z\sqrt{|E|})^{l+1} e^{-z\sqrt{E}} L_{\nu-l-1}^{2l+1}(2z\sqrt{|E|}), \quad (91)$$

where L is the (generalized) Laguerre function and $\nu = e^2/2\sqrt{|E|}$ is a positive integer. Hence the quantization rule is, using $\nu = n+l+1$ where $0\le n$ is the radial quantum number and $1 \le \nu$ the principal quantum number,

$$\Phi(E) = \{n+1+l-[l(l+1)]^{1/2}\}\pi, \quad 0\le n,\ 0\le l. \quad (92)$$

Note that (92) does not have the l degeneracy of the Coulomb problem $\{$since $l-[l(l+1)]^{1/2}$ is never precisely an integer except for $l=0\}$. This degeneracy has been removed because $V(x)$ is similar but not identical to the Coulomb potential.

For case (D),

$$\text{(D)}\ K^2(z) = E + \frac{\lambda e^{-z/\beta}}{1-e^{-z/\beta}} - \frac{b e^{-z/\beta}}{(1-e^{-z/\beta})^2}.$$

For $E<0$, we have

$$S_+ = \int_{z_2}^{z} |K|\,dz \text{ and } S_- = \int_{z_1}^{z} |K|\,dz.$$

These are rather complicated integrals, which can be written in closed form.[18] However, we only need the facts that

$$S_+ \underset{x\to+\infty}{\sim} z\sqrt{|E|},\qquad (z')^{-1/2} \xrightarrow[x\to+\infty]{} 1, \quad (93)$$

and

$$\Phi = \pi\beta[(\lambda-E)^{1/2} - |E|^{1/2} - b^{1/2}].$$

The solutions for $v'' + K^2 v = 0$ which are regular at $z=0$ are[19-21] (AS, Chap. 15)

$$v(z) = e^{-\sigma z/\beta}(1-e^{-z/\beta})^{\rho} F(a, b, 2\rho, 1-e^{-z/\beta}), \quad (94)$$

where

$$\sigma = \beta\sqrt{|E|},\quad \rho = \tfrac{1}{2} + \tfrac{1}{2}(1+4\beta^2 b)^{1/2},\quad a = \sigma+\rho+\beta(\lambda-E)^{1/2},\quad b = \sigma+\rho-\beta(\lambda-E)^{1/2}. \quad (95)$$

Then

$$\psi(x) = (z')^{-1/2} v(z) \underset{x\to+\infty}{\sim} Ae^{-\sigma z/\beta} + Be^{\sigma z/\beta} = Ae^{-S_+} + Be^{-S_-}. \quad (96)$$

Here

$$A = \frac{\Gamma(2\rho)\Gamma(-2\sigma)}{\Gamma(b-2\sigma)\Gamma(a-2\sigma)},\quad B = \frac{\Gamma(2\rho)\Gamma(2\sigma)}{\Gamma(a)\Gamma(b)} \quad (97)$$

and ψ remains finite at plus infinity only if $B=0$, hence only if a or b is a negative integer. Since a is positive, this means

$$b=\sigma+\rho-\beta(\lambda-E)^{1/2}$$
$$=\tfrac{1}{2}+\tfrac{1}{2}(1+4\beta^2 b)^{1/2}+\beta\sqrt{|E|}-\beta(\lambda-E)^{1/2}=-n.$$

Hence

$$\Phi(E)=\pi\beta\,[(\lambda-E)^{1/2}-\sqrt{b}-\sqrt{|E|}\,]$$
$$=\pi[n+\tfrac{1}{2}+\tfrac{1}{2}(1+4\beta^2 b)^{1/2}-\beta\sqrt{b}],$$
$$0\leq n\leq\beta\sqrt{\lambda}-\tfrac{1}{2}-\tfrac{1}{2}(1+4\beta^2 b)^{1/2}. \qquad (98)$$

If we write $\beta^2 b=l(l+1)$, this becomes

$$\Phi(E)=\pi\{n+1+l-[l(l+1)]^{1/2}\},\quad 0\leq n\leq\beta\sqrt{\lambda}-l-1. \qquad (99)$$

Note that this is identical to the quantization rule (92), $K^2(z)$ the Coulomb potential. The effect of the expotential tail instead of the x^{-1} tail is to cut n off at $\beta\sqrt{\lambda}-l-1$, making the number of bound states finite.

V. CONCLUSION

A method has been presented for obtaining the transmission coefficient (T), reflection coefficient (R), phase shifts (μ and ν), and quantization rule for various types of potentials with one and two turning points. To obtain T, R, μ, and ν, one need merely calculate W for the given potential, adjust the parameters in the relevant transformed potential to make z' as constant as possible, and use the formulas given, and similarly for quantization rules.

In addition, an approximate wave function, valid for all x, may be obtained merely by calculating the integral $S(x)=\int^x k\,dx$ and writing the argument z of the transformed wave function as a function of $S(x)$. The wave function is then given in terms of known, generally tabulated functions. It is not clear that this procedure for obtaining $\psi(x)$ is much less work than straightforward integration of the Schrödinger equation—it is certainly no more.

The next step in the approximation scheme is clearly to determine when the approximation is valid. One must take, for each potential, the expression $z(x)$ obtained by neglecting $\langle z;x\rangle$ in (4) and determine that it indeed satisfies the self-consistent requirement

$$|\tfrac{1}{2}\langle z;x\rangle|\ll k^2(x).$$

Since

$$\tfrac{1}{2}\langle z;x\rangle=-(k/K)^{-1/2}\frac{d^2(k/K)^{-1/2}}{dx^2}, \qquad (100)$$

this is analogous to the usual condition for validity of the WKB approximation, $|k'/2k^2|\ll 1$, to which (100) reduces if $K\equiv 1$ and we neglect k''. The condition for validity thus depends both on the mapping we use and on the original potential.

VI. ACKNOWLEDGMENT

It is a pleasure to thank Professor Joseph Mayer for many stimulating conversations and the National Science Foundation for financial support.

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*Work supported by the National Science Foundation.

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