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Rereading Langer's influential 1937 JWKB paper: the unnecessary Langer transformation; the two $\hbar$'s

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Abstract

After making the 'Langer transformation', $r = e^x, \psi(r) = e^{x/2}u(x)$, Langer found the first-order JWKB hydrogen radial wavefunction to be as if the centrifugal potential were $\hbar^2(l+1/2)^2/(2r^2)$, thereby 'justifying' the substitution suggested by Kramers and known to get, in first order, the correct r^{l+1} behavior at the origin, the correct phase shift and the exact energy levels. There have been many extensions of the Kramers–Langer substitution: to get the exact origin behavior at any pre-specified higher order; to show that no substitution is necessary at infinite order; to replace $\hbar^2 l(l+1)$ by $L^2+\hbar L$, with L set equal to $l\hbar$ at the end. Recently, it was discovered that Langer's JWKB solution in x was exactly equivalent to a JWKB solution in r for $r^{-1/2}\psi(r)$: namely the Langer transformation was irrelevant. How can there be many seemingly incompatible JWKB expansions to solve one equation? The key is the ambiguous treatment of $\hbar$: in the radial kinetic energy, $\hbar$ is the expansion parameter; in the centrifugal potential, $\hbar$ is implicit, passive and not expanded. By designating the implicit $\hbar_i$ by its own symbol, one sees immediately how the different JWKB expansions correspond to different partitions of the centrifugal potential between expansion $\hbar$ and implicit $\hbar_i$ and therefore solve different equations. The different expansions represent the same physical solution only when $\hbar_i = \hbar$. Moreover, in the two-$\hbar$ notation, 'the generalization' of the Kramers–Langer substitution is made transparently simple:

$$\hbar^2 l(l+1) \to \hbar_i^2(l+1/2)^2 - \hbar^2/4.$$

That is, the implicit $\hbar_i^2/4$ that completes the square is compensated by the expansion $-\hbar^2/4$ that modifies the second-order JWKB wavefunction directly and higher orders indirectly.

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1. Introduction

In the abstract of his influential 1937 *Physical Review* paper [1], Langer attacked the Jeffreys–Wentzel–Kramers–Brillouin (JWKB) analysis of the radial wave equation as 'uncritical and in error .... When correctly applied the JWKB theory yields the formulas which have been found to be called for on other grounds'. Langer was justifying the substitution empirically suggested by Kramers [2], to replace $l(l+1)$ by $\left(l+\frac{1}{2}\right)^2$ in the centrifugal potential, one consequence of which was to convert the behavior of the JWKB wavefunction at the origin from $r^{\frac{1}{2}+[l(l+1)]^{1/2}}$ to the r^{l+1} of the exact wavefunction [3]. Langer's 'correct application' of the JWKB theory was based on the transformation, $r = \mathrm{e}^x$, $\psi(r) = \mathrm{e}^{x/2}u(x)$, which moved the origin to $-\infty$ and eliminated the second-order pole. The first-order (with respect to $\hbar$) x formulas turned out to be equivalent to first-order r formulas with $l(l+1)$ replaced by $\left(l+\frac{1}{2}\right)^2$. In this 'correct-in-first-order' sense, Langer justified Kramers' substitution, which today is often called the 'Langer substitution' or 'Langer modification' or 'Langer correction' or 'Kramers–Langer ...'.

To see how Langer's transformation might further modify the centrifugal potential beyond first order, Krieger and Rosenzweig [4] in 1967 pushed Langer's x solution to third order. But on transformation back to r, they concluded negatively that 'there is no effective potential [in the r variable] ... which will give rise to the correct result ...'.

Focussing on the wavefunction at the origin and not on Langer's transformation, Beckel and Nakhleh [5] in 1963 found a value K to substitute for $l(l+1)$ so that the third-order (but not first-order) JWKB wavefunction went like r^{l+1}. In 1974, Fröman and Fröman [6] extended Beckel and Nakhleh's idea to each order up to 9th. In 1984, Seetharaman and Vasan [7] found the complete generalization to any specific order and showed moreover that in infinite order K is exactly $l(l+1)$, i.e. no modification. Starting from a JWKB quantization of the angular momentum, Robnik and Salasnich [8] in 1997 and Romanovski and Robnik [9] in 2000 derived formulas equivalent to infinite-order Seetharaman and Vasan, from which Romanovski and Robnik asserted that they had '... thus resolved the controversies about the so-called 'Langer correction' ..., by explaining that by ignoring the 'Langer correction' and assuming the exact value of the quantal angular momentum we indeed get the exact result of the energy spectrum after calculating the terms of all orders and summing the WKB series'.

In 1999, Hainz and Grabert [10] discovered a completely different way to get the r^{l+1} behavior in all orders beyond zeroth by decomposing the centrifugal potential into a zeroth- and first-order term with respect to $\hbar$: $\hbar^2 l(l+1) = L^2 + \hbar L$. (At the end, L is set equal to $\hbar l$.) They concluded that no Langer modification was necessary.

In 2004, the biggest surprise of all came with Dahl and Schleich's observation [11] that the Kramers substitution in Langer's derivation came entirely from the $r^{1/2} = \mathrm{e}^{x/2}$ in $\psi(r) = r^{1/2}u(x)$, and that Langer's exponential transformation was completely irrelevant. Dahl and Schleich concluded insightfully that '... Langer's analysis may, in fact, be considered as nothing more than a somewhat complicated way of solving (the radial wave equation for $r^{-1/2}\psi(r)$) by the JWKB method'. So simple a revelation took 67 years to discover.

How can we unify and compare these seemingly incompatible solutions?

$(l+1/2)^2$ is correct only in first order; there is no generalizing effective potential.

$l(l+1)$ is correct in infinite order.

Intermediate values are correct in between first and infinite order.

$(\hbar l)^2 + \hbar(\hbar l)$ is correct.

$(l+1/2)^2$ is correct for all orders in the equation for $r^{-1/2}\psi(r)$.

The key idea is that there are *two* $\hbar$'s: the $\hbar$ in the radial kinetic energy term is the active, *expansion* $\hbar$; the $\hbar$ buried in the centrifugal potential is passive, implicit, intrinsic, never expanded. The solutions differ in how $\hbar$ is split between expansion parameter and implicit parameter. In consequence, there are many JWKB expansions, not one that the words 'power series in $\hbar$' would seem to imply.

Comparison of the various expansions is enormously simplified by a fortunate fact: in each case the JWKB behavior at $r = 0$ can be solved exactly, before the two $\hbar$'s are set equal.

In two-$\hbar$ notation, 'the generalization' of the Kramers–Langer substitution is near trivial.

2. The original JWKB radial solution

The radial Schrödinger equation for a central potential $V(r)$,

$$\left(-\frac{\hbar^2}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) + \frac{\hbar^2 l(l+1)}{2r^2} - E\right)\psi(r) = 0, \tag{1}$$

has a JWKB solution, valid near $r = 0$, completely specified by

$$\psi_{\mathrm{JWKB}}(r) = \mathrm{e}^{\int q\,dr/\hbar}, \tag{2}$$

$$q = q^{(0)} + \hbar q^{(1)} + \hbar^2 q^{(2)} + \cdots, \tag{3}$$

$$q^{(0)} = +\sqrt{2\left(V(r) + \frac{\hbar^2 l(l+1)}{2r^2} - E\right)}, \tag{4}$$

$$q^{(N)} = -\left(\mathrm{d}q^{(N-1)}/\mathrm{d}r + \sum_{k=1}^{N-1} q^{(k)} q^{(N-k)}\right) \Big/ (2q^{(0)}). \tag{5}$$

Seetharaman and Vasan [7] (and Romanovski and Robnik [9]) solved these equations near $r = 0$ *order-by-order* to obtain

$$\frac{1}{\hbar}(q^{(0)} + \hbar q^{(1)} + \cdots + \hbar^{2N} q^{(2N)}) = \frac{1}{r}\left(\frac{1}{2} + \sqrt{l(l+1)}\sum_{k=0}^{N}[4l(l+1)]^{-k}\binom{\frac{1}{2}}{k}\right) + \mathrm{O}(r^0). \tag{6}$$

In infinite order, $q/\hbar$ sums to $(l+1)/r + \mathrm{O}(r^0)$, and $\psi_{\mathrm{JWKB}}(r) = \mathrm{e}^{\int q\,dr/\hbar} \sim r^{l+1}$.

2.1. Where's the $\hbar$?

The expansion for the exponent of r in ψ_{JWKB} is a series in $[4l(l+1)]^{-1}$ rather than in $\hbar$. What happened to the dependence on $\hbar$? The answer is that the $q^{(2N)}$ depend implicitly on $\hbar$ through the definition of $q^{(0)}$ in (4) in such a way to cancel the explicit factor $\hbar^{2N-1}$. That cancellation can be substantially clarified by notationally distinguishing the two $\hbar$'s.

2.2. Two-$\hbar$ notation and behavior at the origin

The JWKB solution (2)–(5) in fact solves the more general radial Schrödinger equation,

$$\left(-\frac{\hbar^2}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) + \frac{\hbar_i^2 l(l+1)}{2r^2} - E\right)\psi(r) = 0, \tag{7}$$

with (4) replaced by

$$q^{(0)} = +\sqrt{2\left(V(r) + \frac{\hbar_i^2 l(l+1)}{2r^2} - E\right)}, \tag{8}$$

in which $\hbar_i$ denotes an independent, implicit parameter that takes no part in generating the expansion, but that will be set equal to $\hbar$ to recover the physical problem at the end. This notation merely codifies the currently practiced computational details of the JWKB solution of the radial Schrödinger equation. The solution of (7) that is regular at the origin behaves not like r^{l+1} (which it would if $\hbar_i = \hbar$) but instead like

$$\psi(r) \sim r^{\lambda}, \tag{9}$$

where the characteristic exponent $\lambda = \lambda(\hbar, \hbar_i)$ is the (in this case positive) root of the (Frobenius) indicial equation

$$\hbar^2\lambda(\lambda - 1) = \hbar_i^2 l(l+1), \tag{10}$$

$$\lambda(\hbar, \hbar_i) = \frac{1}{2} + \frac{1}{\hbar}\sqrt{\hbar_i^2 l(l+1) + \hbar^2/4} \tag{11}$$

$$= \frac{1}{2} + \frac{\hbar_i}{\hbar}\sqrt{l(l+1)}\sum_{k=0}^{\infty}\left[\frac{\hbar^2}{\hbar_i^2 4l(l+1)}\right]^k \binom{\frac{1}{2}}{k}. \tag{12}$$

Note that (i) the explicit expansion in powers of $\hbar$ for the leading exponent of r at the origin comes out of the indicial equation [12, 13]; (ii) when $\hbar_i$ is set equal to $\hbar$, the termwise $\hbar$-dependence drops out, obscuring the order-by-order identification of the terms; (iii) the first-order JWKB analysis gives the first-order term in (12) correctly, and, although it is not the correct value for the infinite-order solution of the physical problem, it is not 'in error' in the sense of the solution whose characteristic exponent is given by (10)–(12).

3. The Hainz and Grabert decomposition

Even though the original JWKB method is not in error, Kramers saw that different JWKB approaches might be more useful. We see here that they differ in the partition between expansion $\hbar$ and implicit $\hbar_i$. The JWKB expansion discovered by Hainz and Grabert [10] fits neatly into a two-$\hbar$ notation when their 'L' is replaced by '$l\hbar_i$'. Hainz and Grabert's radial Schrödinger equation is, in two-$\hbar$ notation,

$$\left(-\frac{\hbar^2}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) + \frac{\hbar_i^2 l^2 + \hbar\hbar_i l}{2r^2} - E\right)\psi(r) = 0. \tag{13}$$

The centrifugal potential in (13) differs subtly from (7): $\hbar_i^2 l$ is replaced by $\hbar\hbar_i l$, transferring some of the passive $\hbar_i$-dependence of the potential to the expansion $\hbar$. The difference in the small-r behavior is pronounced:

$$\psi(r) \sim r^{\lambda(\hbar,\hbar_i)}, \qquad \lambda(\hbar, \hbar_i) = \frac{\hbar_i l + \hbar}{\hbar}. \tag{14}$$

When $\hbar_i$ is set equal to $\hbar$, the behavior at the origin is r^{l+1} for all orders from the first. The explicit JWKB equations (4) and (5) for $q^{(0)}$ and $q^{(1)}$, respectively, also change slightly:

$$q^{(0)} = +\sqrt{2\left(V(r) + \frac{\hbar_i^2 l^2}{2r^2} - E\right)} \tag{15}$$

$$q^{(1)} = \left(\frac{\hbar_i l}{r^2} - \frac{\mathrm{d}q^{(0)}}{\mathrm{d}r}\right) \Big/ (2q^{(0)}) \tag{16}$$

$$q^{(N)} = -\left(\mathrm{d}q^{(N-1)}/\mathrm{d}r + \sum_{k=1}^{N-1} q^{(k)} q^{(N-k)}\right) \Big/ (2q^{(0)}), \qquad (N \geqslant 2). \tag{17}$$

The practical advantage of Hainz and Grabert is the achievement of r^{l+1} behavior (for $l > 0$) at first and all subsequent orders, versus the infinite series of (12), without a 'contrived' Kramers–Langer substitution.

4. Kramers–Langer–Beckel–Nakhleh–Fröman–Fröman and finite-Seetharaman–Vasan

At first glance, the Beckel–Nakhleh–Fröman–Fröman and finite-Seetharaman–Vasan idea would appear to be the ultimate *ad hoc* single-finite-order 'contrived' substitution. But their idea can be embedded (not uniquely) into a two-$\hbar$ formalism that at infinite order gives an exact solution when the two $\hbar$'s are set equal, perhaps suggesting more than *ad hoc* significance. The omnibus radial equation is

$$\left(-\frac{\hbar^2}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) + \frac{\hbar_i^2 K}{2r^2} + \frac{\hbar^{2N+2}}{\hbar_i^{2N}}\frac{l(l+1) - K}{2r^2} - E\right)\psi(r) = 0. \tag{18}$$

At the origin, the regular solution of (18) goes like $r^{\lambda(\hbar,\hbar_i)}$, with

$$\lambda(\hbar, \hbar_i) = \frac{1}{2} + \frac{\hbar_i\sqrt{K}}{\hbar}\sqrt{1 + \frac{\hbar^2}{4\hbar_i^2 K} + \frac{\hbar^{2N+2}}{\hbar_i^{2N+2}K}(l(l+1) - K)}. \tag{19}$$

No matter what value K has, if $\hbar_i = \hbar$, then in infinite order $\lambda = l + 1$. In use, K is to be evaluated as the root of $\sqrt{K}\sum_{k=0}^{N}(4K)^{-k}\binom{\frac{1}{2}}{k} - \left(l + \frac{1}{2}\right)$, so chosen to make the $2N$th and $(2N+1)$th JWKB wavefunctions behave like r^{l+1} at the origin when $\hbar_i = \hbar$. (Of course, for calculation of the JWKB wavefunction through order $2N+1$, the term proportional to $\hbar^{2N+2}$ in the potential makes no contribution.) The case $N = 0$ has $K = \left(l + \frac{1}{2}\right)^2$ (Kramers–Langer). The case $N = 1$ is Beckel–Nakhleh. The cases $N = 2$ to $N = 4$ are Fröman and Fröman. $N > 4$ is Seetharaman–Vasan.

5. Dahl and Schleich's revelation

Langer sought to avoid both the finite end point and singular nature of the origin by moving it to $-\infty$ with the transformation, $r = \mathrm{e}^x$. To eliminate the consequent first-derivative $\mathrm{d}/\mathrm{d}x$ term he introduced the $r^{1/2}$ factor, $\psi(r) = r^{1/2}u(x)$. As if by magic, the centrifugal potential changed to $\hbar^2(l + 1/2)^2/2r^2$. Dahl and Schleich, who were familiar with radial Schrödinger equations in arbitrary dimensions, recognized that the important step in Langer's derivation

was the $r^{1/2}$, with analogy to a two-dimensional radial Schrödinger equation. That is, by taking out the factor $r^{1/2}$, (1) is transformed into

$$\left(-\frac{\hbar^2}{2}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)+V(r)+\frac{\hbar^2(l+1/2)^2}{2r^2}-E\right)r^{-1/2}\psi(r)=0, \tag{20}$$

which displays the Kramers expression for the centrifugal potential, albeit with a 'two-dimensional' kinetic energy. Dahl and Schleich correctly point out that a JWKB expansion of (20) is the direct way to get what Langer attempted indirectly through his transformed variable x. There was no necessity to avoid dealing directly with $r = 0$. There was no necessity for the Langer exponential transformation.

The two-$\hbar$ form of Dahl and Schleich is

$$\left(-\frac{\hbar^2}{2}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)+V(r)+\frac{\hbar_i^2(l+1/2)^2}{2r^2}-E\right)r^{-1/2}\psi(r)=0, \tag{21}$$

At the origin, the regular solution goes like

$$\psi\sim r^{\lambda(\hbar,\hbar_i)},\qquad \lambda(\hbar,\hbar_i)=\frac{1}{2}+\frac{\hbar_i}{\hbar}\left(l+\frac{1}{2}\right), \tag{22}$$

which, with $\hbar_i = \hbar$, gives the r^{l+1} behavior for ψ in zeroth and all subsequent orders.

6. Generalization of the Kramers–Langer modification

There is extra insight gained by putting Dahl and Schleich's two-dimensional equation into one-dimensional form. Multiply (21) by $r^{1/2}$ and cancel. The result

$$\left(-\frac{\hbar^2}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+V(r)+\frac{\hbar_i^2(l+1/2)^2}{2r^2}-\frac{\hbar^2}{8r^2}-E\right)\psi(r)=0 \tag{23}$$

is the sought-after 'generalization' of the Kramers–Langer substitution. Contrasted with (7), $\hbar_i^2/8r^2$ has been moved into the implicit $\hbar_i$-dependent potential, and a compensating $-\hbar^2/8r^2$ assigned to the expansion $\hbar$. When Krieger and Rosenzweig [4] ruled an effective potential impossible, they clearly did not consider an expansion-$\hbar$ term. Once the dual role of $\hbar$ in the radial JWKB equation has been unmasked, this generalization is obvious. Note that the $N = 0$ version of (18) given above is indeed just (23).

The explicit operational JWKB equations (4) and (5) for $q^{(0)}$ and $q^{(2)}$, respectively, change slightly because of the $\hbar^2$ term in the potential:

$$q^{(0)}=+\sqrt{2\left(V(r)+\frac{\hbar_i^2(l+1/2)^2}{2r^2}-E\right)} \tag{24}$$

$$q^{(2)}=-\left(\mathrm{d}q^{(1)}/\mathrm{d}r+q^{(1)2}+\frac{1}{4r^2}\right)\Big/(2q^{(0)}) \tag{25}$$

$$q^{(N)}=-\left(\mathrm{d}q^{(N-1)}/\mathrm{d}r+\sum_{k=1}^{N-1}q^{(k)}q^{(N-k)}\right)\Big/(2q^{(0)}),\qquad (N\neq 0,2). \tag{26}$$

Equation (23) and Dahl and Schleich's (21) are completely equivalent, with one-to-one correspondence of the term-by-term solutions. Equation (22) holds for both. A minor advantage of (23)–(26) is their standard form.

Table 1. Characteristic exponent $\lambda(\hbar, \hbar_i)$ for the various radial JWKB wavefunctions.

JWKB variation	$\lambda(\hbar, \hbar_i)$
Original	$\frac{1}{2} + \frac{1}{\hbar}\sqrt{\hbar_i^2 l(l+1) + \hbar^2/4}$
Hainz–Grabert	$\frac{\hbar_i l + \hbar}{\hbar}$
Kramers–Langer–Beckel–Nakhleh–Fröman–Fröman and finite-Seetharaman–Vasan	$\frac{1}{2} + \frac{\hbar_i\sqrt{K}}{\hbar}\sqrt{1 + \frac{\hbar^2}{4\hbar_i^2 K} + \frac{\hbar^{2N+2}}{\hbar_i^{2N+2}K}(l(l+1) - K)}$
Dahl–Schleich and generalized Kramers–Langer	$\frac{1}{2} + \frac{\hbar_i}{\hbar}\left(l + \frac{1}{2}\right)$

7. Explicit JWKB expansion at $r = 0$

The effective potentials discussed here all have the form

$$V_{\text{eff}}(r, \hbar, \hbar_i) = V(r) + \frac{a\hbar_i^2 + b\hbar_i\hbar + c\hbar^2(\hbar/\hbar_i)^{2k}}{2r^2}, \tag{27}$$

where

$$a + b + c = l(l+1), \tag{28}$$

so that

$$V_{\text{eff}}(r, \hbar, \hbar) = V(r) + \frac{\hbar^2 l(l+1)}{2r^2}. \tag{29}$$

Kawai and Takei [13] (proposition 3.6) have proven a general result whose restriction to $V_{\text{eff}}(r, \hbar, \hbar_i)$ is: if $a\hbar_i^2 + b\hbar_i\hbar + c\hbar^2 \neq 0$, and $V(r)$ has at most a first-order pole at $r = 0$, then $q(r)$ has a simple pole at $r = 0$ with a residue equal to $\hbar$ times the characteristic exponent $\lambda(\hbar, \hbar_i)$. Explicitly,

$$q = \frac{q_{-1}(\hbar, \hbar_i)}{r} + \mathrm{O}(r^0), \tag{30}$$

$$\frac{q_{-1}(\hbar, \hbar_i)}{\hbar} = \frac{1}{2} + \frac{1}{\hbar}\sqrt{a\hbar_i^2 + b\hbar_i\hbar + c\hbar^2(\hbar/\hbar_i)^{2k} + \frac{\hbar^2}{4}} \tag{31}$$

$$= \lambda(\hbar, \hbar_i). \tag{32}$$

Our analysis of the behavior of the JWKB radial solutions has been based on (30)–(32), and the various λ are summarized in table 1. Seetharaman and Vasan [7], Romanovski and Robnik [9] and Hainz and Grabert [10] all derived special cases of (30) and (31), JWKB-term by JWKB-term.

That the JWKB expansion gives the correct behavior at $r = 0$ is not trivial. Consider, for instance, the Coulomb potential. When $l = 0$ in both the original JWKB radial solution and in the Hainz–Grabert solution, q does not have a simple pole at $r = 0$, but instead the singular, square-root-type branch-point behavior characteristic of a linear turning point. In this case, the JWKB expansion does not exhibit the correct r^λ behavior at $r = 0$.

With respect to the $l = 0$ case, we note that Koike [14, 15] has developed the exact JWKB analysis for potentials with simple poles, and he has applied it [16] to the Coulomb

potential problem to cover both the original JWKB method and the additional cases that $q^{(0)2} = -2/r - 2E$ and $q^{(0)2} = -2E$. In particular, the $-2/r - 2E$ case includes as a subcase the $l = 0$ case of the original method.

8. Hydrogen atom energy levels

Knowing that one motivation for Kramers–Langer-like substitutions was to get the hydrogen energies correct, the reader might be curious why energies have so far been absent from the discussion. The reason is that the hydrogen atom JWKB energy levels (in units where charge and mass have the value 1) are given by the unified formula,

$$E = -\frac{1}{2\hbar^2(n_r + \lambda(\hbar, \hbar_i))^2}, \qquad (n_r = 0, 1, 2, \ldots), \tag{33}$$

with the details carried by the $\lambda(\hbar, \hbar_i)$. The λ have already been determined from the indicial equations by virtue of Aoki *et al* [12, 13] in (12), (14), (19) and (22), and in table 1. For completeness, a brief derivation of (33) will now be sketched.

For hydrogen, $V = -1/r$. The JWKB solutions that individually satisfy the boundary condition at 0 or at ∞ match, when continued by connection formulas to the classically allowed region, if, and only if [17],

$$\oint_\gamma q\mathrm{d}r/\hbar = 2n_r\pi\mathrm{i}, \qquad (n_r = 0, 1, 2, \ldots). \tag{34}$$

For each case discussed above (except for the unmodified $l = 0$ case [16], which we omit), there is a positive value of K for which

$$q^{(0)}(r) = \sqrt{\frac{K\hbar_i^2}{r^2} - \frac{2}{r} - 2E}\,, \tag{35}$$

so that all the cases can be treated together. The two real zeros of $q^{(0)}(r)$ (the classical turning points) lie on the positive r axis. γ denotes a closed path that encloses both of them, but not the origin. We fix the phase so that $q^{(0)}(r)$ is real and positive between $r = 0$ and the left turning point, which makes $q^{(0)}(r)$ real and negative between the right turning point and $r = +\infty$.

From the Riccati equations generating $q^{(N)}$ and the choice of phase:

$$q^{(0)} = -\sqrt{-2E} + \frac{1}{r\sqrt{-2E}} + \mathrm{O}(r^{-2}) \qquad \text{as} \quad r \to \infty, \tag{36}$$

$$q^{(N)} = \mathrm{O}(r^{-N-1}) \qquad \text{as} \quad r \to \infty, \qquad (N \geqslant 1). \tag{37}$$

The only finite singularities of $q^{(N)}$ are poles at, or square-root-type branch cuts joining, the two classical turning points, and a simple pole in q at the origin [12, 13]. Consequently, each $q^{(N)}$ has a convergent Laurent series for $|r|$ greater than the right turning point, and, via sufficiently large R, $\oint_\gamma q\mathrm{d}r/\hbar$ can be expressed as a sum of residues:

$$\oint_\gamma q\,\mathrm{d}r/\hbar = \oint_{|r|=R} q\,\mathrm{d}r/\hbar - \oint_{|r|=1/R} q\,\mathrm{d}r/\hbar \tag{38}$$

$$= -2\pi\mathrm{i}(\text{residue of } q/\hbar \text{ at } \infty + \text{residue of } q/\hbar \text{ at } 0). \tag{39}$$

The residue at 0 is $\lambda(\hbar, \hbar_i)$ as in (32). From (36) and (37), the residue at ∞ is $-(\hbar\sqrt{-2E})^{-1}$. The energy formula (33) then follows from (34) and (39).

If the hydrogen atom is confined inside a spherical box, then (34) gains an order-dependent phase shift, as discussed in a numerical study of the Hainz–Grabert decomposition by Sinha [18], and (33) no longer holds. The authors thank the referee for this reference.

9. The different expansions, numerical usefulness, and Borel summability

When $\hbar_i \neq \hbar$, the different JWKB expansions solve different radial Schrödinger equations and represent different functions. The $\lambda(\hbar, \hbar_i)$ are all different. When $\hbar_i = \hbar$, the different JWKB expansions solve the same radial Schrödinger equation and represent the same function (e.g., the $\lambda(\hbar, \hbar)$ all equal $l + 1$), but term-by-term they are different. Since JWKB expansions are asymptotic, there are built-in practical restrictions to the length of partial sums and numerical accuracy; the faster the initial convergence, the more useful the expansion. The main motivation for the Kramers–Langer and subsequent substitutions is for more accurate low-order partial sums.

We note that while the JWKB expansion in $\hbar$ is a singular perturbation [19], the implicit $\hbar_i$ is not being used as a perturbation parameter, either regular or singular. It is merely a spectator.

If these JWKB expansions are Borel summable [12, 16, 20–25], then each expansion would be uniquely associated with an analytic function of $\hbar$ (and $\hbar_i$). These different analytic functions would coincide with the physical solution when $\hbar_i = \hbar$. No JWKB expansion would be 'correct' at the expense of the others, although certainly some may be more convenient than others. Computational implementation of Borel summation would permit higher numerical accuracy by inclusion of higher order terms than is possible with partial summation [26, 27].

10. Discussion

The Kramers–Langer substitution has been invaluable for first-order JWKB applications of the radial Schrödinger equation, but its justification has nothing to do with the Langer transformation. The $\left(l+\frac{1}{2}\right)^2$ in Langer's 'derivation' is now known to have come from factoring $r^{1/2}$ out of the wavefunction; the simultaneous replacement of $\mathrm{d}^2/\mathrm{d}r^2$ by $\mathrm{d}^2/\mathrm{d}r^2 + (1/r)\,\mathrm{d}/\mathrm{d}r$ [11] would have ended the question of what next after first order. The question would instead have become, why and how are the two JWKB expansions different. But that realization was recent, and in the intervening years other JWKB expansions were devised, and the original expansion was shown to give the correct behavior at the origin and the correct energy eigenvalues in infinite order. The question then changes to why and how these several JWKB expansions are different, yet represent the same solution of the radial Schrödinger equation.

The key to answering the question is the realization that $\hbar$ has been dealt with ambiguously. $\hbar$ is both expansion parameter and fixed parameter in the definition of the centrifugal contribution to an effective potential. By appropriate labeling of the implicit parameter $\hbar_i$, the various JWKB radial expansions are seen to be solutions of different Schrödinger equations that differ in the partition of the centrifugal potential between expansion $\hbar$ and implicit $\hbar_i$. In particular, the simplest way to understand the Kramers–Langer substitution in an exact context is the radial Schrödinger Equation (23) in which $\hbar^2 l(l+1)$ has been partitioned $\hbar_i^2(l + 1/2)^2 - \hbar^2/4$. The various JWKB expansions all represent the same physical solution when $\hbar_i = \hbar$, although term-by-term the expansions are different.

Langer's equations are not mathematically incorrect, but his explanations and manipulations are misleading. For instance, when $q^{(0)}$ has a simple pole at $r = 0$, the single-exponential JWKB wavefunctions behave correctly at the origin; Dunham's matching condition is valid; and nothing is gained by mapping the origin to $-\infty$. In fairness, Langer worked when the JWKB method was a bridge between classical and quantum mechanics, when usefulness meant how well the low-order JWKB wavefunction matched the exact, when the error estimates were the most important tool, when the dual role of $\hbar$ hid beneath the surface and when the Borel summation hid perhaps even deeper.

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