On the JWKB expansion and Borel summability, with particular attention to modifications of the radial Schrödinger equation

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Approximation and extrapolation of sequences and convergent and divergent series

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JWKB – asymptotic power series in $\hbar$ – and Borel summability for a simple (Airy-function) case

$$\psi_{\text{left}}(x, \hbar) = S(x, \hbar)^{-1/2} \sin \left( \frac{S(x, \hbar)}{\hbar} + \frac{\pi}{4} - \delta \right)$$

$$S(x, \hbar) = S^{(0)}(x) + \hbar^2 S^{(1)}(x) + \hbar^4 S^{(2)}(x) + \cdots$$

$S(0, \hbar)$ by partial summation:
semi-log plot of term magnitudes

$S(0, \hbar)$ by Borel-sum approximant:
semi-log plot of term magnitudes
JWKB and Borel summability: transmission through a barrier for a simple (Airy-function) case

\[ S(x, \hbar) \sim S^{(0)}(x) + \hbar^2 S^{(1)}(x) + \hbar^4 S^{(2)}(x) + \cdots \]

\[ = \frac{1}{\hbar} \int_0^\infty e^{-t/\hbar} \left( S^{(0)}(x) + S^{(1)}(x) \frac{t^2}{2!} + S^{(2)}(x) \frac{t^4}{4!} + \cdots \right) dt \]

asymptotic expansion

equality

Borel transform

Partial sum, 4th order

Borel sum, 4th order

Exact
The radial Schrödinger equation: Langer’s influential 1937 JWKB paper and the unnecessary Langer transformation; the ambiguous ħ; the power of Borel summation


*On the connection formulas and the solutions of the wave equation*

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PART 2. THE RADIAL WAVE EQUATION
Part 2 deals with the radial wave equation for motion in a central field of force. Both the attractive and repulsive Coulomb field are considered. It is shown that the application of the W. K. B. analysis to this equation as it has generally been made is uncritical and in error. The solution commonly identified thereby as the wave function is in fact not the wave function. The “failure” of the W. K. B. formulas, and the apparent necessity for modifying them by replacing the number \( l(l+1) \) by \((l+\frac{1}{2})^2\), has been noted by many investigators. This is traced to the misapplication of the theory. When correctly applied the theory naturally yields the formulas which have been found to be called for on other grounds.
The problem, simply put: focus on behavior at $r = 0$

$$\psi_{\text{exact}}(r, \hbar) \sim r^{l+1}, \text{ as } r \to 0$$

$$\psi_{\text{JWKB}}(r, \hbar) \sim r^{\lambda}, \text{ as } r \to 0$$

$$\lambda = \frac{1}{2} + \sqrt{l(l + 1)}, \text{ in first order of JWKB}$$

$$\neq l + 1$$

$$E_{\text{exact}} = -\frac{1}{2\hbar^2(n_r + l + 1)^2}, \quad (n_r = 0, 1, 2, \ldots)$$

$$E_{\text{JWKB}} = -\frac{1}{2\hbar^2(n_r + \lambda)^2}, \quad (n_r = 0, 1, 2, \ldots)$$

Kramers’ (1926) fix:

$$l(l + 1) \rightarrow \left( l + \frac{1}{2} \right)^2$$

$$\lambda \rightarrow l + 1$$
Langer’s “justification” of Kramers’ modification

\[ r = e^x \]
\[ u(x, \hbar) = r^{-1/2} \psi(r, \hbar) \]

\[ 0 \leq r < \infty \quad \rightarrow \quad -\infty < x < \infty \]

\[ -\frac{\hbar^2}{2} \frac{d^2 \psi}{dr^2} = \left( E - V(r) - \frac{l(l + 1)\hbar^2}{2r^2} \right) \psi \]

\[ \rightarrow -e^{-2x} \frac{\hbar^2}{2} \frac{d^2 u}{dx^2} = \left( E - V(e^x) - \frac{(l + \frac{1}{2})^2\hbar^2}{2e^{2x}} \right) u \]

In first order:
\[ \psi = r^{1/2}u \sim r^{l+1} \]

\[ E_n = -\frac{1}{2\hbar^2(n_r + l + 1)^2}, \quad n_r = 0, 1, 2, \ldots \]

which is identical with the results of substituting

\[ \left( l + \frac{1}{2} \right)^2 \quad \text{for} \quad l(l + 1) \quad \text{in the original} \quad \psi(r, \hbar) \quad \text{equation.} \]
What about orders 2, 3, ... , $\infty$?

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

is not the same as

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

How do you generalize the Kramers-Langer substitution to get the right answer in infinite order?
The main developments after Langer’s paper:

- Krieger and Rosenzweig (1967): no effective potential
- Beckel and Nakhleh (1963): $l(l+1)\rightarrow K$, correct for 2nd order
- Fröman and Fröman (1974): $l(l+1)\rightarrow K$, correct for 9th order
- Seetharaman and Vasan (1984): $l(l+1)\rightarrow K$, correct for 2nd through $\infty$
- Robnik and Salasnich (1997)
- Romanovski and Robnik (2000)
- Hainz and Grabert (1999): $\hbar^2 l(l+1)\rightarrow L^2 + \hbar L$
- Dahl and Schleich (2004): it’s the $r^{-1/2}$ in $r^{-1/2}\psi$

\[
-\frac{\hbar^2}{2} \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) r^{-1/2}\psi + \left( V(r) + \frac{\hbar^2(l + \frac{1}{2})^2}{2r^2} - E \right) r^{-1/2}\psi = 0
\]
The centrifugal potential in the original scheme is really
\[
\frac{l(l+1)\hbar_i^2}{2r^2}
\]
where \(\hbar_i\) is a second, independent parameter, set equal to \(\hbar\) after the JWKB expansion has been generated.

The centrifugal potentials of the various schemes all have the form,
\[
\frac{a\hbar_i^2 + b\hbar_i\hbar + c\hbar^{2+k}\hbar_i^{-k}}{2r^2}
\]
When \(\hbar_i\) is set equal to \(\hbar\), the two-\(\hbar\) potential is the physical one:
\[
\frac{(a + b + c)\hbar^2}{2r^2} = \frac{l(l+1)\hbar^2}{2r^2}
\]
Centrifugal potentials in two-$\hbar$ notation

\[
\frac{a\hbar_i^2 + b\hbar_i\hbar + c\hbar^{2+k}\hbar_i^{-k}}{2r^2}
\]

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Centrifugal Potential</th>
</tr>
</thead>
</table>
| Original | \[
\frac{l(l+1)\hbar_i^2}{2r^2}
\] |
| Kramers-Langer-Beckel-Nakhleh-Fröman-Fröman and finite-Seetharaman-Vasan | \[
K\hbar_i^2 + \hbar^2 \left( \frac{\hbar}{\hbar_i} \right)^{2N} \left[ l(l+1) - K \right] \frac{1}{2r^2}
\] |
| Hainz-Grabert | \[
\frac{l^2\hbar_i^2 + l\hbar_i\hbar}{2r^2}
\] |
| Dahl-Schleich | \[
\frac{(l+1/2)^2\hbar_i^2 - \hbar^2/4}{2r^2}
\] |
Characteristic exponents are all \( l+1 \) when \( \hbar_i = \hbar \).

<table>
<thead>
<tr>
<th>Scheme</th>
<th>( \lambda(\hbar,\hbar_i) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original</td>
<td>( \frac{1}{2} + \frac{1}{\hbar} \sqrt{l(l+1)\hbar_i^2 + \hbar^2 / 4} )</td>
</tr>
<tr>
<td>Kramers-Langer-Beckel-Nakhleh-Fröman-Fröman and finite-Seetharaman-Vasan</td>
<td>( \frac{1}{2} + \frac{1}{\hbar} \sqrt{K\hbar_i^2 + \hbar^2 / 4 + \hbar^2 (\hbar / \hbar_i)^{2N} [l(l+1) - K]} )</td>
</tr>
<tr>
<td>Hainz-Grabert</td>
<td>( \frac{l\hbar_i + \hbar}{\hbar} )</td>
</tr>
<tr>
<td>Dahl-Schleich and generalized Kramers-Langer</td>
<td>( \frac{1}{2} + \frac{\hbar_i}{\hbar} \left( l + \frac{1}{2} \right) )</td>
</tr>
</tbody>
</table>
THE “generalization” in two-$\hbar$ notation

$$\left( -\frac{\hbar^2}{2} \frac{d^2}{dr^2} + V(r) + \frac{\hbar_i^2 (l + \frac{1}{2})^2}{2r^2} - \frac{1}{4} \hbar^2 - E \right) \psi(r) = 0$$

Equivalent to Dahl-Schleich, but as an equation for $\psi$, not $r^{-1/2}\psi$
in two-$\hbar$ notation
The centrifugal potential for physical reasons is taken as zeroth order, requiring an implicit $\hbar_i$.

The different JWKB methods differ in how $\hbar$ is partitioned between expansion $\hbar$ and implicit $\hbar_i$. These different sums only coincide with each other and with the physical solution when $\hbar_i = \hbar$, but even then, term-wise, they are different.

If each method is Borel summable, then there is no unique correct partition. All are correct. Some may be more useful than others. Some may be better candidates to bridge classical and quantum mechanics than others. (Some are more equal than others?)
Borel summability of the various JWKB radial wave functions

\[ \psi_{\text{JWKB}}(r) = N(\hbar) \phi(r) e^{S^{(0)}(r)/\hbar} \left( 1 + f^{(1)}(r)\hbar + f^{(2)}(r)\hbar^2 + f^{(3)}(r)\hbar^3 + \cdots \right) \]

To prove Borel summability, have to construct the Borel sum of the power series factor and show that the resulting function is a solution of the Schrödinger equation with the correct boundary conditions.

\[
\left( 1 + f^{(1)}(r)\hbar + f^{(2)}(r)\hbar^2 + f^{(3)}(r)\hbar^3 + \cdots \right) = \frac{1}{\hbar} \int_0^\infty e^{-t/\hbar} \left( 1 + f^{(1)}(r) \frac{t}{1!} + f^{(2)}(r) \frac{t^2}{2!} + f^{(3)}(r) \frac{t^3}{3!} + \cdots \right) dr
\]
Exact solution of the various modified two-$\hbar$ radial Schrödinger equations: *eigenfunctions*

The *energy eigenfunctions* are specified via $\lambda = \lambda(\hbar, \hbar_i)$

$$\psi_{n_r}(r, \hbar) = r^\lambda L_{n_r}^{(2\lambda-1)} \left( \frac{2r}{\hbar^2(n_r + \lambda)} \right) e^{-\frac{r}{\hbar^2(n_r + \lambda)}}$$

$$E_{n_r} = -\frac{1}{2\hbar^2(n_r + \lambda)^2}, \quad (n_r = 0, 1, 2, 3, \ldots)$$

Note: $\lambda = \lambda(\hbar, \hbar_i)$
Exact solution of the various modified two-\(\hbar\) radial Schrödinger equations: *arbitrary energy*

This is the general case where Borel summability is pertinent. Focus on the solution that satisfies the boundary condition at \(\infty\). The exact solution is a Whittaker \(W\) confluent hypergeometric function that has a *useful integral representation*.

\[
\begin{align*}
\eta &= \left(-2E\right)^{-1/2} \\
\psi &= W_{\frac{\eta}{\hbar},\lambda-rac{1}{2}}\left(\frac{2r}{\hbar\eta}\right) \\
&= e^{-\frac{r}{\hbar\eta}} \left(\frac{2r}{\hbar\eta}\right)^\lambda \frac{1}{\Gamma\left(-\frac{\eta}{\hbar} + \lambda\right)} \int_0^\infty e^{-\frac{2r}{\hbar\eta}t} t^{-\frac{\eta}{\hbar}+\lambda-1} (1 + t)^{\frac{\eta}{\hbar}+\lambda-1} \, dt
\end{align*}
\]
Hainz-Grabert case: simplest integrand

\[ \lambda - 1 = \frac{\bar{h} l}{\hbar} = \frac{k}{\bar{h}} \]

\[ W \frac{\eta}{\bar{h}}, \frac{1}{2} + \frac{k}{\bar{h}} \left( \frac{2r}{\hbar \eta} \right) = -e^{-\frac{r}{\hbar \eta}} \left( \frac{2r}{\hbar \eta} \right)^{1+k/\hbar} \frac{\Gamma \left( \frac{\eta-k}{\hbar} \right)}{2\pi i} \]

\[ \times \int_{(\infty, 0^+, e^{2\pi i \infty})} e^{-\frac{2r}{\hbar \eta} t} \left( e^{-\pi i t} \right) \frac{k-\eta}{\hbar} (1 + t) \frac{k+\eta}{\hbar} \, dt \]

Evaluate by saddle-point method
Saddle-point expansion results:

The saddle-point occurs at

\[ t_0 = - \left( \frac{1}{2} - \frac{k\eta}{2r} - \frac{\sqrt{r^2 - 2r\eta^2 + k^2\eta^2}}{2r} \right) \]

The integration contour passes through the saddle-point vertically, as if from \( t_0 + i\infty \) to \( t_0 - i\infty \).

The saddle point expansion has the form,

\[ \psi = \psi_{\text{leading asymptotic form}} \times \left( 1 + \sum_{j=1}^{\infty} a_j(r)h^j \right) \]

The expansion is unique and therefore is the JWKB expansion, up to normalization.
The saddle-point expansion does not lead backwards to the original integral!

The saddle-point integration picks out even powers of $t$:

$$i \int_{i\infty}^{-i\infty} e^{t^2/\hbar} \left(1 + at + bt^2 + \cdots\right) dt = \sqrt{\pi\hbar} \left(1 - \frac{1}{2}b\hbar + \cdots\right)$$

Possible solution:
1. Make second integral representation reflecting $t$ through $t_0$.
2. Both go through the same saddle point. Take half the sum.
3. Difficulty: integration paths different. Can be made to coincide on the imaginary axis, but need a convergence factor.
Conclusions and remarks

The two-$\hbar$ Hainz-Grabert (and Dahl-Schleich) versions of the radial JWKB Schrödinger equation are proved Borel summable by using a saddle-point expansion of a standard integral representation of the Whittaker confluent hypergeometric function and subsequent manipulations.

The other versions are likely to be Borel summable, but the proof will require a convergent expansion superimposed on the divergent expansion because of the square-root entanglement of the two $\hbar$'s. (work in progress)

Not discussed is the “normalization constant” of the JWKB expansion and the proportionality of the JWKB solution to the Whittaker function. There are two such normalization constants: turning point vs. normalization at $\infty$, and either vs. the Whittaker function. These are non-trivial, but doable.

The Borel summability of the modified JWKB radial coulomb wave functions makes rigorous the two-$\hbar$ analysis of the several-radial-JWKB methods and provides confidence in the validity of these modified methods to potentials where proof of Borel summability would be more difficult.
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