On WKB Series for the Radial Kepler Problem

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We obtain the rigorous WKB expansion to all orders for the radial Kepler problem, using the residue calculus in evaluating the WKB quantization condition in terms of a complex contour integral in the complexified coordinate plane. The procedure yields the exact energy spectrum of this Schrödinger eigenvalue problem and thus resolves the controversies around the so-called "Langer correction". The problem is nontrivial also because there are only a few systems for which all orders of the WKB series can be calculated, yielding a convergent series whose sum is equal to the exact result, and thus sheds new light to similar and more difficult problems.

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In recent years many studies have been devoted to systematical investigation of the accuracy of semiclassical approximations, which is a very important problem, especially in the context of quantum chaos (Casati and Chirikov 1995, Gutzwiller 1990, Robnik 1998). Among them the WKB expansions to all orders for a one dimensional system with the potential $V(x) = U_0/\cos^2(\alpha x)$ was investigated by Robnik and Salasnich (1997a) and for the angular momentum operator by Robnik and Salasnich (1997b) and by Salasnich and Sattin (1997). An important earlier classic paper is by Bender et al (1977). It has been shown for the potentials treated in the above papers that all WKB orders can be obtained, that the semiclassical series for the eigenvalues converges and when summed yields the well known exact results. In the present paper we apply the same WKB method to the radial Kepler problem. We solve the problem in a rigorous way, using the residue calculus in evaluating the complex contour integrals in order to obtain all orders in the $\hbar$-expansion, which confirms the conjecture by Robnik and Salasnich (1997b) about the form of all WKB terms in this problem. When summed, the WKB series yields the exact energy spectrum of the Kepler problem.

The problem is very important as it resolves the controversies around the so-called "Langer correction" (Langer 1937, Gutzwiller 1990), which states that in applying the first (leading) order WKB method (the torus quantisation of Einstein and Maslov) one should replace the exact value of the angular momentum $L = l(l+1)\hbar$ by $L = (l + \frac{1}{2})^2\hbar$, in which case we then get (by brute force) the exact result for the Coulomb energy spectrum. Of course, as explained by Robnik and Salasnich (1997b), this "Langer correction" has no physical foundation and indeed is just an ad hoc guess. Indeed, they have shown that higher order terms in the Kepler (Coulomb) energy eigenvalue problem exactly compensate the error done by the "Langer correction", so that after summing up the infinite WKB series we get the exact result free of any ad hoc assumptions like "Langer correction". Thus, the importance of the present paper is to provide a rigorous proof of the hypothesis (ansatz) of Robnik and Salasnich (1997b) on this problem. We shall consider the Schrödinger equation in the complex-
ified coordinate space and shall use the standard WKB ansatz. Then we solve the quantisation condition (which is equivalent to the single-valuedness condition of the wavefunction in the complexified coordinate plane) by using the residue calculus. The problem is not trivial, because it is hard to guess the correct form of the polynomial terms that enter the quantisation condition at each order, and experience in problems connected to the polynomial differential equations (Dolichanin et al 1998) proved to be crucial. In fact, using this experience we went further producing the more general results on WKB method in the Hamiltonian systems with one degree of freedom which will be presented in a separate paper (Robnik and Romanovski 1999).

We consider the Schrödinger equation for the radial Kepler problem

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

where

\[ V(r) = \frac{L^2}{2r^2} - \frac{\alpha}{r} \]  

with \( L^2 = l(l+1)h^2, l = 0, 1, 2, \ldots \), being the squared angular momentum, and \( \alpha > 0 \).

We can always write the wavefunction as

\[ \psi(r) = \exp \left\{ \frac{i}{\hbar} \sigma(r) \right\} \]  

where the phase \( \sigma(r) \) is a complex function that satisfies the differential equation

\[ \sigma'^2(r) + \left(\frac{\hbar}{i}\right) \sigma''(r) = 2(E - V(r)). \]  

The WKB expansion for the phase is

\[ \sigma(r) = \sum_{k=0}^{\infty} \left(\frac{\hbar}{i}\right)^k \sigma_k(r). \]  

Substituting (3) into (4) and comparing like powers of \( \hbar \) gives the recursion relation

\[ \sigma'^2 + \left(\frac{\hbar}{i}\right) \sigma'' + 2(E - V(r)) = 0. \]  

The quantization condition is obtained by requiring the uniqueness of the wavefunction, so for the contour integral around a closed contour in the complexified coordinate plane \( r \) we must have

\[ \oint_{\gamma} d\sigma = \sum_{k=0}^{\infty} \left(\frac{\hbar}{i}\right)^k \oint_{\gamma} d\sigma_k = 2\pi n_r \hbar, \]  

where \( n_r \geq 0 \), an integer number, is the radial quantum number and \( \gamma \) is a complex contour enclosing the turning points on the real axis.

The zero-order term is given by

\[ \oint_{\gamma} d\sigma_0 = 2 \oint_{\gamma} \sqrt{2(E - V(r))} = \alpha \pi \sqrt{\frac{2}{-E} - 2\pi L} \]  

and the first odd term is

\[ \left(\frac{\hbar}{i}\right)^1 \oint_{\gamma} d\sigma_1 = -\pi \hbar. \]  

¿From (6) we get

\[ \sigma'_2 = (L^4 - 6\alpha L^2 r + (3\alpha^2 - 12L^2 E)r^2 + 8\alpha Er^3)/(8r(\sqrt{2Er^2 + 2\alpha r - L^2})^3) \]  

and

\[ \sigma'_3 = (3r(\alpha^2 r^2 + 2\alpha Er(-5L^2 + 4Er^2) + \alpha^2(-3L^2 + 4Er^2) - 2EL^2(L^2 + 8Er^2)))/(8(\sqrt{2Er^2 + 2\alpha r - L^2})^8). \]  

Computing also \( \sigma'_4 \) one finds, correspondingly (Robnik and Salasnich 1997b),

\[ \left(\frac{\hbar}{i}\right)^2 \oint_{\gamma} d\sigma_2 = -\hbar^2 \pi \frac{1}{4L} \]  

and

\[ \left(\frac{\hbar}{i}\right)^4 \oint_{\gamma} d\sigma_4 = \hbar^4 \frac{\pi}{64L^3}. \]  

¿From this result the following general formula for the \( \hbar^{2k} \) term

was conjectured (Robnik and Salasnich 1997b), \( k = 1, 2, 3, \ldots \)

\[ \left(\frac{\hbar}{i}\right)^{2k} \oint_{\gamma} d\sigma_{2k} = -2\pi \hbar \left(\frac{\hbar}{i}\right)^k 2^{-2k} \lambda^{1-2k} \]  

(14)
and so, taking into account that due to the conjecture of Bender at al (1977)
\[ \int \gamma \, d\sigma_{2k+1} = 0, \tag{15} \]
we get
\[ \frac{\alpha}{\sqrt{-2E}} = \hbar\left[(nr + \frac{1}{2}) + \sum_{k=0}^{\infty} \left(\frac{k}{2}\right)2^{-2k}\lambda^{1-2k}\right], \tag{16} \]
where \( \lambda = L/\hbar = \sqrt{l(l+1)} \), implying the energy spectrum for the quantal Kepler problem \([\text{1}], \text{2}\).

\[ E = \frac{-\alpha^2}{2\hbar^2(nr + l + 1)^2}. \tag{17} \]

We will show that formulae \([\text{14}], \text{15}\) indeed hold. To compute the contour integrals \([\text{7}]\)
\[ \int \gamma \, d\sigma_k \tag{18} \]
we find the form of the functions \(\sigma'_k\). We have from \([\text{8}]\)
\[ \sigma'_0 = \sqrt{\frac{2Er^2 + 2\alpha r - L^2}{r^2}} = \frac{\sqrt{2Er^2 + 2\alpha r - L^2}}{r}. \tag{19} \]

We see that \(\sigma'_0\) is a two valued function. However we can cut the complex plane along the real axis between the turning points \(r_1, r_2\) (\(r_1 < r_2\)), which are the roots of the equation
\[ 2Er^2 + 2\alpha r - L^2 = 0 \tag{20} \]
and in such case we obtain a single valued function in the cutting plane. Then from \([\text{9}]\) we get
\[ \sigma'_1 = \frac{\sqrt{\alpha r - L^2}}{2r(\sqrt{2Er^2 + 2\alpha r - L^2})^2}. \tag{21} \]

We now make an "educated guess" concerning the form of the coefficients \(\sigma'_k\). Namely, we shall show that the formulae \(\text{(22)}\)–\(\text{(24)}\) are crucial for our analysis, however it is not obvious from the first few expressions for \(\sigma'_k\) that this shape of the coefficients contains exactly the information which we need. It is interesting to mention that similar recurrence relations arise in the investigation of the famous problem of ordinary differential equations, the so-called center-focus problem (Dolichanin et al 1998, eq.(15)), and our previous experience turned out to be very helpful here. Our surmise reads then:
\[ \sigma'_{2s} = \frac{P_{4s-1}}{r(\sqrt{2Er^2 + 2\alpha r - L^2})^{6s-1}}, \tag{22} \]
and
\[ \sigma'_{2s+1} = \frac{rQ_{4s-1}}{(\sqrt{2Er^2 + 2\alpha r - L^2})^{6s+2}}, \tag{23} \]
where \(s > 0\), the degrees of polynomials \(P_{4s-1}, Q_{4s-1}\) (as functions of \(r\)) are not greater than \(4s - 1\), and \(P_{4s-1}\) has the form
\[ P_{4s-1} = \frac{1}{2^{2s}}(\frac{1}{s})(L^{4s} - 6L^{4s-2}\alpha sr + \ldots). \tag{24} \]

Here and below we denote by \(Q_k\) any polynomial of degree less than or equal to \(k\).

We prove the formulae \((\text{22})\)–\(\text{(24)}\) by induction on \(s\). According to \([\text{10}], \text{11}\) we see that for \(s = 1\) the statements are true. Let us suppose that they are proven for all \(s < m\) and consider the case \(s = m\).

To compute \(\sigma'_{2m}\) using the recurrence formula \([\text{13}]\) we note that
\[ \frac{\sigma'_{2k+1}\sigma'_{2(m-k-1)+1}}{\sigma'_0} = \frac{r^3Q_{4k-1}Q_{4m-4k-5}}{(\sqrt{2Er^2 + 2\alpha r - L^2})^{6m-1}} \tag{25} \]
\[ = \frac{r^4Q_{4m-6}}{r(\sqrt{2Er^2 + 2\alpha r - L^2})^{6m-1}}, \]
\[ \frac{\sigma'_{2m+1}\sigma'_{2(m-1)+1}}{\sigma'_0} = \frac{r^2(\alpha r - L^2)Q_{4m-5}}{r(\sqrt{2Er^2 + 2\alpha r - L^2})^{6m-1}} \tag{26} \]
and
\[
\frac{\sigma_{2m-1}'}{\sigma_0'} = \frac{1}{\sigma_0'} \left( \frac{r Q_{4m-5}}{(\sqrt{2Er^2 + 2\alpha r - L^2})^{6m-4}} \right)'
\]
for \(r^2 | (-L^2 + 6\alpha r - 6\alphamr + 10Er^2 - 12Emr^2)Q_{4m-5} + r(-L^2 + 2\alpha r + Er^2) \times Q'_{4m-5})/(r(\sqrt{2Er^2 + 2\alpha r - L^2})^{6m-1}).\)

Thus we see that the fractions \((24) - (27)\) have the form \((22)\) and the polynomials in the numerators have no influence on the two lowest terms of the numerator of \(\sigma_{2m}'\).

Therefore
\[
\sigma_{2m}' = -\sum_{k=1}^{m-1} \frac{\sigma_{2k}' \sigma_{2(m-k)}'}{2\sigma_0'} + \frac{r^2 Q_{4m-3}}{r(\sqrt{2Er^2 + 2\alpha r - L^2})^{6m-1}} - \sum_{k=1}^{m-1} \frac{P_{4k-1} P_{4(m-k)-1} + r^2 Q_{4m-3}}{2r(\sqrt{2Er^2 + 2\alpha r - L^2})^{6m-1}}.
\]

Note that the degree of the polynomials \(P_{4k-1} P_{4(m-k)-1}\) is less or equal \(4m - 2\). Hence it remains to compute the two lowest terms of the polynomial \(\sigma_{2m}'\). Observing now that
\[
P_{4k-1} P_{4(m-k)-1} = \frac{1}{22m} \left( \frac{1}{k} \right) \left( \frac{1}{m-k} \right) \times (L_{4m}^4 - 6mAr L_{4m-2}^2 + \ldots)
\]
we get from \((28)\)
\[
\sigma_{2m}' = \frac{L_{4m}^4 - 6L_{4m-2}^2 mAr + r^2 Q_{4m-3}}{22m+1r(\sqrt{2Er^2 + 2\alpha r - L^2})^{6m-1}} \times \sum_{k=1}^{m-1} \left( \frac{1}{k} \right) \left( \frac{1}{m-k} \right).
\]

Therefore, taking into account the equality
\[
\sum_{k=0}^{m} \left( \frac{1}{k} \right) \left( \frac{1}{m-k} \right) = 0
\]
(which is just a special case of the Vandermonde’s convolution, see e.g. (Graham et al 1994)) we conclude that \((22)\) holds.

It remains to find \(\sigma_{2m+1}'\). We get
\[
-\frac{\sigma_{1}' \sigma_{2m}'}{\sigma_0'} - \frac{\sigma_{2m}'^2}{2\sigma_0'} = \frac{(6om + 12Emr)P_{4m-1} + (L^2 - 2\alpha r - 2Er^2) \times P_{4m-1}')/(2(\sqrt{2Er^2 + 2\alpha r - L^2})^{6m+2})
\]
and in the case \(0 < k < m\) we have
\[
\frac{\sigma_{2k}' \sigma_{2(m-k)+1}'}{\sigma_0'} = \frac{r P_{4k-1} Q_{4m-4k-1}}{(\sqrt{2Er^2 + 2\alpha r - L^2})^{6m+2}}.
\]

Using the induction assumptions \((22)\) and \((24)\) we conclude that \((22), (23)\) are of the form \((22)\), so each \(\sigma_{2m}'\) obeys \((22)\).

Now we can compute the integrals \((18)\). We are going to use the residue calculus. The integration contour in our complex \(r\) plane (complexification of the coordinate space \(r\) ) is chosen so that it encircles the two turning points \(r_1\) and \(r_2\). They are connected by a cut so that each \(\sigma_m'\) is single-valued, and has singularities (poles) either at infinity or at \(r = 0\). Hence the integration contour encircles now the poles that lie outside the integration contour and, therefore, the calculation becomes very easy. Namely, using the residue theorem we get
\[
\int_{\gamma} \left( \frac{h}{i} \right)^{2k} i \, d\sigma_{2k} = 2\pi i \left( \frac{h}{i} \right)^{2k} (\text{Res}_0 \sigma_{2k}' + \text{Res}_\infty \sigma_{2k}').
\]
\(\bar{\gamma}\) from \((22), (24)\) it is easily seen
\[
\text{Res}_0 \sigma_{2k}' = i \left( \frac{1}{22k^2} \right) \left( \frac{1}{k} \right).
\]

For large \(r\) we have according to \((22)\) the convergent series
\[
\sigma_{2k}' = \frac{P_{4k-1}}{r(\sqrt{2Er^2 - 1 + \frac{\alpha}{Er} - \frac{L^2}{2Er^2}})^{6k-1}}
\]
\[
\frac{P_{4k-1}}{r(r\sqrt{2E})^{6k-1}} \times [1 + (6k-1)\left(\frac{\alpha}{Er} - \frac{L^2}{2E r^2}\right) + \ldots].
\]

and, therefore,

\[\text{Res}_{\infty} \sigma'_2k = 0.\] (37)

Similarly, we obtain

\[\oint_{\gamma} d\sigma_{2k+1} = 0,\] (38)

since \(r = 0\) is not a singular point of \(\sigma'_2k+1\) and

\[\text{Res}_{\infty} \sigma'_2k+1 = 0.\] (39)

Hence

\[
\left(\frac{\hbar}{i}\right)^{2k} \oint_{\gamma} d\sigma_{2k} = \left(2\pi i\right)^k \hbar^{2k} \left(\frac{i}{\left(-1\right)^k 2^{2k} L^{2k-1}} \left(\frac{1}{k}\right)\right) = -2\pi \hbar \frac{\lambda^{1-2k}}{2k} \left(\frac{1}{k}\right).
\]

Thus formulae (14), (15) and (16) are proven, resulting in the exact energy spectrum (17).

In conclusion, we have shown that the residue theorem can be successfully applied in computing the WKB series of certain potentials in one degree of freedom, in particular for the Kepler (Coulomb) potential. In this way we have confirmed the conjecture by Robnik and Salasnich (1997b) about the form of all the terms in the corresponding WKB expansion and thus resolved the controversies about the so-called "Langer correction" (Langer 1937, Gutzwiller 1990), by explaining that by ignoring the "Langer correction" and assuming the exact value of the quantal angular momentum we indeed get the exact result for the energy spectrum after calculating the terms of all orders and by summing the WKB series (after completing our work the preprint by Hainz and Grabert (1999) with similar result (but another convergent WKB expansion) was posted).

It appears interesting to apply this method to the investigation of other potentials like, for example, the above mentioned potential, \(V = U_0/\cos^2(\alpha x)\). Here the difficulties arise because the integrated function has infinitely many singular points.

The most important problem in this context is the general formulation of the exact WKB quantization condition in terms of contour integrals for arbitrary one-dimensional potentials.

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