Semiclassical Expansion for the Angular Momentum

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After reviewing the WKB series for the Schrödinger equation we calculate 
the semiclassical expansion for the eigenvalues of the angular momentum
operator. This is the first systematic semiclassical treatment of the angular
momentum for terms beyond the leading torus approximation.

1 Introduction

The semiclassical method of torus quantization is just the first term of a
certain $\hbar$-expansion, usually called the WKB expansion. The method goes
back to the early days of quantum mechanics and was developed by Bohr
and Sommerfeld for one-freedom systems and separable systems, it was then
generalized for integrable (but not necessarily separable) systems by Einstein
[1], which is called EBK or torus quantization. In fact, Einstein’s result
was corrected for the phase changes due to caustics by Maslov [2,3], but the
torus quantization formula thus obtained is still just a first term in the WKB
expansion, whose higher terms can be calculated with a recursion formula in
one degree systems, but are generally unknown in systems with more than
one degree of freedom.

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Our goal in the present paper is to generalize the WKB expansion of the Schrödinger equation to the angular momentum operator. To the best of our knowledge a detailed analysis of this problem has not been undertaken in the literature so far. Thus our present work is the first systematic semiclassical expansion of the angular momentum problem.

In section 2 we treat the one-dimensional stationary Schrödinger equation by analyzing the corrections to the leading torus quantization term, and in the section 3 we study the solutions of the angular momentum operator by calculating the corrections to the leading torus quantization term. In section 4 we discuss the results and draw some general conclusions.

2 WKB expansion for the Schrödinger equation

We consider the one-dimensional stationary Schrödinger equation

\[
\left(-\frac{\hbar^2}{2} \frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x),
\]

where \(V(x)\) is a potential with two turning points. We can always write the wave function as

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

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

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

The WKB expansion for the phase is

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

Substituting (4) into (3) and comparing like powers of \(\hbar\) gives the recursion relation \((n > 0)\)

\[
\sigma_0'' = 2(E - V(x)), \quad \sum_{k=0}^{n} \sigma_k' \sigma_{n-k} + \sigma_{n-1}'' = 0.
\]
The quantization condition is obtained by requiring the uniqueness of the wave function
\[ \oint d\sigma = \sum_{k=0}^{\infty} \left( \frac{\hbar}{i} \right)^k \oint d\sigma_k = 2\pi n\hbar , \]
where \( n \geq 0 \), an integer number, is the radial quantum number.

The zero order term, which gives the Bohr-Sommerfeld formula, is given by
\[ \oint d\sigma_0 = 2 \int dx \sqrt{2(E - V(x))} , \]
and the first odd term in the series gives the Maslov corrections (Maslov index is equal to 2)
\[ \left( \frac{\hbar}{i} \right) \oint d\sigma_1 = -\pi \hbar . \]

All the other odd terms vanish when integrated along the closed contour because they are exact differentials [4]. So the quantization condition can be written
\[ \sum_{k=0}^{\infty} \left( \frac{\hbar}{i} \right)^{2k} \oint d\sigma_{2k} = 2\pi(n + \frac{1}{2})\hbar , \]
thus a sum over even-numbered terms only. The next two non-zero terms are [4,5]
\[ \left( \frac{\hbar}{i} \right)^2 \oint d\sigma_2 = -\hbar^2 \frac{1}{12} \frac{\partial^2}{\partial E^2} \int dx \frac{V''(x)}{\sqrt{2(E - V(x))}} , \]
\[ \left( \frac{\hbar}{i} \right)^4 \oint d\sigma_4 = \hbar^4 \left( \frac{1}{240} \frac{\partial^3}{\partial E^3} \int dx \frac{V'''(x)}{\sqrt{2(E - V(x))}} - \frac{1}{576} \frac{\partial^4}{\partial E^4} \int dx \frac{V''(x)V''(x)}{\sqrt{2(E - V(x))}} \right) . \]

So we have obtained the first two quantum corrections to the torus quantization for the one-dimensional stationary Schrödinger equation. We note that higher-order corrections quickly increase in complexity and only in a few cases a systematic WKB expansion can be worked out even explicitly to all orders, resulting in a convergent series whose sum is identical to the exact spectrum [4,6,7].
3 Semiclassical expansion for the angular momentum

We consider the eigenvalue equation of the angular momentum

\[ \hat{L}^2 Y(\theta, \phi) = \lambda^2 \hbar^2 Y(\theta, \phi) , \]  

(12)

where \( \hat{L}^2 \) is formally given by the equation

\[ \hat{L}^2 = \hat{P}^2_\theta + \frac{\hat{P}^2_\phi}{\sin^2(\theta)} , \quad P_\phi = L_z , \]  

(13)

with

\[ \hat{P}^2_\theta = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \cot(\theta) \frac{\partial}{\partial \theta} \right) , \]  

(14)

\[ \hat{P}^2_\phi = -\hbar^2 \frac{\partial^2}{\partial \phi^2} . \]  

(15)

We can write the eigenfunction as

\[ Y(\theta, \phi) = T(\theta)e^{in_\phi} , \]  

(16)

and we obtain

\[ \hat{P}^2_\phi Y(\theta, \phi) = n^2 \hbar^2 Y(\theta, \phi) , \]  

(17)

and also

\[ T''(\theta) + \cot(\theta)T'(\theta) + (\lambda^2 - \frac{n^2}{\sin^2(\theta)})T(\theta) = 0 . \]  

(18)

Notice that \( \hbar \) does not appear in this equation anymore. To perform the WKB expansion we introduce a small parameter \( \epsilon \), which might be thought of as proportional to \( \hbar \), and consider the eigenvalue problem

\[ \epsilon^2 T''(\theta) + \epsilon^2 \cot(\theta)T'(\theta) = Q(\theta)T(\theta) , \]  

(19)

where

\[ Q(\theta) = W(\theta) - \lambda^2 = \frac{n^2}{\sin^2(\theta)} - \lambda^2 . \]  

(20)
Thus small $\epsilon$ limit is equivalent to the large $n_\phi$ and/or large $\lambda$ limit. The parameter $\epsilon$ helps to organize the WKB series; we set $\epsilon = 1$ when the calculation is completed. First we put

$$ T(\theta) = \exp \left( \frac{1}{\epsilon} S(\theta) \right) , $$

where $S(\theta)$ is a complex function that satisfies the differential equation

$$ S'^2(\theta) + \epsilon S''(\theta) + \epsilon \cot(\theta)S'(\theta) = Q(\theta) . $$

The WKB expansion for the function $S(\theta)$ is given by

$$ S(\theta) = \sum_{k=0}^{\infty} \epsilon^k S_k(\theta) , $$

and by comparing like powers of $\epsilon$ we obtain a recursion formula ($n > 0$)

$$ S'^2_0 = Q, \quad \sum_{k=0}^{n} S'_k S'_{n-k} + S''_{n-1} + \cot(\theta)S'_{n-1} = 0 . $$

Straightforward calculations give for the first few terms

$$ S'_0 = -\frac{1}{2} Q^\frac{1}{2} , $$

$$ S'_1 = -\frac{1}{4} Q'Q^{-1} - \frac{1}{2} \cot(\theta) , $$

$$ S'_2 = -\frac{1}{32} Q'^2 Q^{-5/2} - \frac{1}{8} \frac{d}{d\theta}(Q'Q^{-3/2}) - \frac{1}{8} \cot^2(\theta)Q^{-1/2} $$

$$ - \frac{1}{4} \left( \frac{d}{d\theta} \cot(\theta) \right) Q^{-1/2} . $$

The exact quantization of the wave function is given by

$$ \int dS = \sum_{k=0}^{\infty} \int dS_k = 2\pi i n_\theta , $$

where we have now set $\epsilon = 1$. This integral is a complex contour integral which encircles the two turning points on the real axis. Obviously, it is
derived from the requirement of the uniqueness of the complex wave function \( T \) [4,6].

The zero order term is given by

\[
\oint dS_0 = 2i \int d\theta \sqrt{\lambda^2 - W(\theta)} = 2\pi i (\lambda - n_\phi), \tag{29}
\]

and the first term reads

\[
\oint dS_1 = -\frac{1}{4} \ln Q|_{\text{contour}} = -\pi i. \tag{30}
\]

Evaluating \( \ln Q \) once around the contour gives \( 4\pi i \) because the contour encircles two simple zeros of \( Q \).

All the other odd terms vanish when integrated along the closed contour because they are exact differentials [4]. So the quantization condition can be written as

\[
\sum_{k=0}^{\infty} \oint dS_{2k} = 2\pi i n_\theta + \frac{1}{2}, \tag{31}
\]

and thus it is a sum over even–numbered terms only. The next non–zero term is given by

\[
\oint dS_2 = -i \left( \frac{1}{12} \frac{\partial^2}{\partial (\lambda^2)^2} \int d\theta \frac{W''(\theta)}{\sqrt{\lambda^2 - W(\theta)}} + \frac{1}{2} \frac{\partial}{\partial (\lambda^2)} \int d\theta \frac{W'(\theta) \cot(\theta)}{\sqrt{\lambda^2 - W(\theta)}} \right) + \frac{1}{4} \int d\theta \frac{\cot^2(\theta)}{\sqrt{\lambda^2 - W(\theta)}}. \tag{32}
\]

In all integrals the limits of integration are between the two turning points. After substitution \( z = \tan (\theta) \), we have

\[
\int d\theta \frac{W''(\theta)}{\sqrt{\lambda^2 - W(\theta)}} = \frac{4n_\phi^3}{\sqrt{\lambda^2 - n_\phi^2}} \int dz \frac{(1 + z^2)}{z^6} \sqrt{\frac{z^2}{z^2 - \beta}} = \frac{3\pi}{2n_\phi} (\lambda^2 - n_\phi^2) + 2\pi n_\phi (\lambda^2 - n_\phi^2) = \tag{33}
\]

where \( \beta = n_\phi^2 / (\lambda^2 - n_\phi^2) \), so that

\[
\frac{\partial^2}{\partial (\lambda^2)^2} \int d\theta \frac{W''(\theta)}{\sqrt{\lambda^2 - W(\theta)}} = \frac{3\pi}{n_\phi}. \tag{34}
\]
For the other integrals we use the same procedure.

\[ \int d\theta \frac{W''(\theta) \cot (\theta)}{\sqrt{\lambda^2 - W(\theta)}} = - \frac{2n^2_\phi}{\sqrt{\lambda^2 - n^2_\phi}} \int dz \frac{1}{z^2} \sqrt{\frac{z^2}{z^2 - \beta}} = - \frac{\pi}{n_\phi} (\lambda^2 - n^2_\phi), \]  
(35)

from which we obtain

\[ \frac{\partial}{\partial (\lambda^2)} \int d\theta \frac{W'(\theta) \cot (\theta)}{\sqrt{\lambda^2 - W(\theta)}} = - \frac{\pi}{n_\phi}. \]  
(36)

The last integral gives

\[ \int d\theta \frac{\cot^2 (\theta)}{\sqrt{\lambda^2 - W(\theta)}} = \frac{1}{\sqrt{\lambda^2 - n^2_\phi}} \int dz \frac{1}{z^2(1 + z^2)} \sqrt{\frac{z^2}{z^2 - \beta}} = \pi (\frac{1}{n_\phi} - \frac{1}{\lambda}). \]  
(37)

In conclusion

\[ \oint dS_2 = -i \left( \frac{1}{12} \frac{3\pi}{n_\phi} + \frac{1}{2} \left( \frac{\pi}{n_\phi} \right) + \frac{1}{4} \frac{\pi}{n_\phi} - \frac{1}{\lambda} \right) = \frac{\pi i}{4\lambda}, \]  
(38)

where, importantly, the \( n_\phi \) dependence drops out now. Thus up to the second order in \( \epsilon \) the quantization condition reads

\[ \lambda + \frac{1}{8\lambda} = l + \frac{1}{2}, \]  
(39)

where \( l = n_\theta + n_\phi \). The term \( 1/8\lambda \) is the first quantum correction to the quantization of the angular momentum. From this result we can argue ("conjecture by educated guess") that the \( \epsilon^{2k} \) term in the WKB series is \( (k > 0) \)

\[ \oint dS_{2k} = 2\pi i \left( \frac{1}{2} \right) \frac{1}{k} 2^{-2k} \lambda^{1-2k}, \]  
(40)

so that the WKB expansion of the angular momentum to all orders is given by

\[ \sum_{k=0}^{\infty} \left( \frac{1}{2} \right) \frac{1}{k} 2^{-2k} \lambda^{1-2k} = l + \frac{1}{2}. \]  
(41)

This is the exact formula for the relationship between \( l \) and \( \lambda \), because

\[ \sum_{k=0}^{\infty} \left( \frac{1}{2} \right) \frac{1}{k} 2^{-2k} \lambda^{1-2k} = \frac{1}{2} \sqrt{1 + 4\lambda^2}, \]  
(42)
and the equation $\sqrt{1 + 4\lambda^2/2} = l + 1/2$ can be inverted and gives $\lambda = \sqrt{l(l+1)}$. This completes our investigation of the semiclassical expansion for the angular momentum, where it remains in general to prove the conjectured formula for $k \geq 2$.

4 Discussion and conclusions

In the present paper we offer the first calculation of the higher WKB terms beyond the torus quantization leading terms for the angular momentum.

This analysis explains the exactness of the torus quantization for the entire 3-dim Kepler problem. As is well known, the 3-dim Kepler problem can be reduced to a 1-dim radial problem with potential $V(x) = \frac{L^2}{2x^2} - \frac{1}{x}$, where $L$ is the angular momentum. Since the problem is separable, the wave functions (for the angular momentum and for the radial part) multiply and their phases have the additivity property, and therefore the total phase written as $\frac{i}{\hbar}(\sigma - i\hbar S)$ must obey the quantization condition (uniqueness of the wave function). As shown by the authors in [8], the quantum corrections (i.e. terms higher than the torus quantization terms) do indeed compensate mutually term by term, and only the torus quantization terms remain.

One important future project is to analyze a more general class of the 1-dim potentials and to extend results to integrable but not separable systems with two or more degrees of freedom.

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