Accuracy of Semiclassical Methods for Shape Invariant Potentials

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Abstract

We study the accuracy of several alternative semiclassical methods by computing analytically the energy levels for many large classes of exactly solvable shape invariant potentials. For these potentials, the ground state energies computed via the WKB method typically deviate from the exact results by about 10%, a recently suggested modification using nonintegral Maslov indices is substantially better, and the supersymmetric WKB quantization method gives exact answers for all energy levels.

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1. Introduction

A variety of semiclassical methods have been proposed and used for determining the energy levels of one-dimensional potentials. The standard WKB method is discussed in most quantum mechanical texts \cite{1, 2} but there are several recently suggested modifications based on supersymmetric quantum mechanics \cite{3}, energy dependent phase losses at the classical turning points with nonintegral Maslov indices \cite{4}, and other related approaches \cite{5}. As expected, all semiclassical methods yield good energy eigenvalues $E_n$ for large values of the quantum number $n$. However, their accuracy varies quite substantially for small values of $n$ depending on the choice of potential. Also, many potentials only have a small number of bound states, so that the possibility of considering large values of $n$ does not exist. In this paper, we make a stringent test of the accuracy of various semiclassical methods by computing the eigenenergies of the ground state and other low lying states for many large classes of potentials which have the property of shape invariance \cite{6} under supersymmetry transformations. We have chosen shape invariant potentials since (i) they are exactly solvable and all eigenvalues are explicitly known; (ii) the integrals appearing in the semiclassical quantization conditions can all be performed analytically; (iii) the nonintegral Maslov indices used in the recent semiclassical approach \cite{4} of Friedrich and Trost (FT) can be expressed in terms of superpotentials. Our plan is to first review three semiclassical approaches and the main ideas involving shape invariant potentials. We will then compute the quantization condition integrals analytically and determine energy eigenvalues. The results are presented in Tables 1 and 2, and we give some concluding remarks on the accuracy of various semiclassical approaches.

2. Semiclassical Quantization Conditions

(i) WKB Quantization: The usual form of the semiclassical energy quantization condition (in units of $\hbar = 2m = 1$) is \cite{1, 2}

$$
\int_{x_L}^{x_R} dx \sqrt{E - V(x)} = (n + \frac{\mu}{4}) \pi , \quad \mu = \frac{\phi_L + \phi_R}{\pi/2} , \quad (n = 0, 1, 2, \ldots) ,
$$

where the classical turning points $x_L$ and $x_R$ are given by $V(x_L) = V(x_R) = E$. The Maslov index $\mu$ denotes the total phase loss during one period in units of $\pi/2$. It contains contributions from the phase losses $\phi_L$ and $\phi_R$ due to reflections at the left and right classical turning points $x_L$ and $x_R$ respectively. In the standard WKB approach, one takes $\phi_L = \phi_R = \pi/2$, and an integer Maslov index $\mu = 2$ for all energy levels. This gives the familiar result $(n + \frac{1}{2})\pi$ for the right hand side of the WKB quantization condition.

(ii) SWKB Quantization: Another semiclassical approach \cite{3} which has been widely studied in recent years is based on the ideas of supersymmetric quantum mechanics \cite{9}. Here, the supersymmetric partner potentials $V_-(x)$ and $V_+(x)$ are given in terms of the superpotential $W(x)$ by
\[ V_\pm = W^2(x) \pm W'(x). \] For the case of unbroken supersymmetry, \( V_-(x) \) and \( V_+(x) \) have degenerate energy levels except that \( V_-(x) \) has an additional level at \( E_0^{-} = 0 \). The corresponding ground state wave function \( \psi_0^-(x) \) is related to the superpotential \( W(x) \) via

\[ W(x) = -\frac{\psi_0^-(x)'}{\psi_0^-(x)}; \quad \psi_0^-(x) \propto e^{-\int_x^x' dx' W(x')} . \tag{2} \]

The supersymmetric WKB (SWKB) approach [3] results from combining the ideas of supersymmetry with the lowest order WKB method. The SWKB quantization condition is

\[ \int_{x_L'}^{x_R'} dx \sqrt{E^{-} - W^2(x)} = n\pi, \quad (n = 0, 1, 2, \ldots) , \tag{3} \]

where the two turning points \( x_L' \) and \( x_R' \) are given by \( W(x) = \pm \sqrt{E^{-}} \). Note that for \( n = 0 \), the turning points coincide and the SWKB quantization condition gives the exact result \( E_0^{-} = 0 \) for the ground state energy.

(iii) Friedrich-Trost Quantization: This very recent proposal [4] makes use of the standard quantization condition [eq. (1)] with nonintegral, energy-dependent Maslov indices \( \mu \). More specifically, the phase loss is taken to be given by

\[ \tan(\frac{\phi_L}{2}) = \frac{\psi'(x_L)}{k\psi(x_L)}, \quad \tan(\frac{\phi_R}{2}) = -\frac{\psi'(x_R)}{k\psi(x_R)} , \tag{4} \]

where \( k \equiv \sqrt{E - V_{\text{min}}} \) and \( V_{\text{min}} \) is the minimum value of the potential \( V(x) \). In Ref. [4], it was suggested that one could use the lowest order WKB wave function in eq. (4) in order to determine the phase losses \( \phi_L, \phi_R \) for any practical application. Indeed, it was shown that for power law potentials \( x^p \) with \( p = 4, 5, 6 \), this method gave better numerical results for the ground state energies than the standard WKB method, and also substantially improved wave functions.

The FT approach of using the WKB wave function in eq. (4) is rather cumbersome. It can be significantly simplified for the ground state by using eq. (4). The phase losses \( \phi_L, \phi_R \) can then be re-written as

\[ \tan(\frac{\phi_L}{2}) = -\frac{W(x_L)}{k}, \quad \tan(\frac{\phi_R}{2}) = \frac{W(x_R)}{k} . \tag{5} \]

In this paper, we will assume eq. (5) to be valid for all energy levels in computing eigenenergies by the FT approach.

3. Shape Invariant Potentials

Given a superpotential \( W(x, a_0) \) depending on a set of parameters \( a_0 \), the supersymmetric partner potentials \( V_\pm(x, a_0) \) are given by

\[ V_\pm(x, a_0) = W^2(x, a_0) \pm W'(x, a_0) . \tag{6} \]
These partner potentials are shape invariant if they both have the same $x$-dependence $Upton a \ a_1 = f(a_0)$ and an additive constant $R(a_0)$. The shape invariance condition is

$$V_+(x, a_0) = V_-(x, a_1) + R(a_0) \ .$$

This special property permits an immediate analytic determination of energy eigenvalues [6] and eigenfunctions [7]. For unbroken supersymmetry, the eigenvalues are

$$E_0^{(-)} = 0 \ , \ E_n^{(-)} = \sum_{k=0}^{n-1} R(a_k) \ .$$

Many aspects of the bound states and scattering matrices of shape invariant potentials have been studied [9] including several choices [10] for the change of parameters $a_1 = f(a_0)$. In this paper, we confine our attention to shape invariant potentials corresponding to a translational change of parameters.

4. Computation of Energy Eigenvalues

All known families of shape invariant potentials in which the change of parameters is a translation $a_1 = a_0 + \beta$ are listed in Table 1. Names of the potentials and the corresponding superpotentials are given. Also tabulated is the minimum value $V_{-\min}$ of the potential $V_-(x)$ and the position $x_{\min}$ of the minimum. Subtracting $V_{-\min}$ from $V_-(x)$ yields the tabulated potential $V(x)$, whose minimum value is clearly $V_{\min} = 0$. The exact energy eigenvalues $E_n^{exact}$ for $V(x)$ coming from eq. (8) are also given.

To assess the accuracy of various semiclassical approaches, the first step is to evaluate the two types of integrals appearing in the quantization conditions. We denote the integral in the WKB condition eq. (1) by $I_{WKB}$ and the integral in the SWKB condition eq. (3) by $I_{SWKB}$. The integrals can be handled analytically using contour integration in the complex plane taking special care of the singularities at infinity and the cut going between the turning points. The results are given in Table 1 in terms of the following expressions:

$$I_1(a, b) \equiv \int_a^b dy \sqrt{(y-a)(b-y)} = \frac{\pi}{8}(b-a)^2 \ ;$$

$$I_2(a, b) \equiv \int_a^b dy \frac{dy}{y} \sqrt{(y-a)(b-y)} = \frac{\pi}{2}(a+b) - \pi \sqrt{ab} \ , (0 < a < b) \ ;$$

$$I_3(a, b) \equiv \int_a^b \frac{dy}{y^2+1} \sqrt{(y-a)(b-y)} = \frac{\pi}{\sqrt{2}} \left[ \sqrt{1+a^2} \sqrt{1+b^2} - ab + 1 \right]^{1/2} - \pi \ ;$$

$$I_4(a, b) \equiv \int_a^b \frac{dy}{1-y^2} \sqrt{(y-a)(b-y)} = \frac{\pi}{2} \left[ 2 - \sqrt{(1-a)(1-b) - (1+a)(1+b)} \right] , (-1 < a < b < 1) \ ;$$
\[ I_5(a, b) \equiv \int_a^b \frac{dy}{y^2 - 1} \sqrt{(y - a)(b - y)} = \frac{\pi}{2} [\sqrt{(a + 1)(b + 1)} - \sqrt{(a - 1)(b - 1) - 2}] , (1 < a < b) ; \]

In all the above integrals, the limits \( a, b \) are real numbers with \( a < b \). We have given explicit expressions for the above integrals since they are not easily available in standard integration tables.

Once \( I^{WKB} \) and \( I^{SWKB} \) have been computed, one can apply the quantization conditions to see how accurate the WKB, SWKB and FT approaches are. For the WKB and SWKB approaches, it is possible to get complete analytic results - these are shown in Table 1. The FT approach is also mostly analytical, but the final computations need numerical work. Results corresponding to specific numerical choices of the parameters appearing in the potentials are shown in Table 2.

As an illustrative example, consider the Rosen-Morse II (hyperbolic) potential, for which the superpotential is

\[ W(x) = A \tanh \alpha x + \frac{B}{A} . \]

With a change of variables \( y = \tanh \alpha x \), the SWKB integral is

\[ I^{SWKB} = \frac{A}{\alpha} \int_{y'_L}^{y'_R} \frac{dy}{1 - y^2} \sqrt{[-y^2 - \frac{2B}{A^2} + (\frac{E}{A^2} - \frac{B^2}{A^4})]} \]

with turning points given by \( Ay' + \frac{B}{A} = \pm E^{(-)} \). One then sees that the integral is \( \frac{A}{\alpha} I_4(y'_L, y'_R) \).

Substitution into the SWKB quantization condition \( I^{SWKB} = n\pi \) and solving for \( E^{(-)} \) gives

\[ E^{(-)SWKB}_n = A^2 - (A - n\alpha)^2 + \frac{B^2}{A^2} - \frac{B^2}{(A - n\alpha)^2} \]

which is the exact answer for all energy levels! Similar steps give the WKB integral to be \( I^{WKB} = \frac{\sqrt{A(A + \alpha)}}{\alpha} I_4(y'_L, y'_R) \) where the turning point are given by

\[ A(A + \alpha)y^2 + 2By + (\frac{B^2}{A(A + \alpha)} - E) = 0 . \]

Substitution into the WKB quantization condition \( I^{WKB} = (n + \frac{1}{2})\pi \) and solving for the energy gives

\[ E^{WKB}_n = A(A + \alpha) - (\sqrt{A(A + \alpha)} - \frac{\alpha}{2} - n\alpha)^2 + \frac{B^2}{A(A + \alpha)} - \frac{B^2}{(\sqrt{A(A + \alpha)} - \frac{\alpha}{2} - n\alpha)^2} \]

The WKB approach does not give the exact eigenvalues. The full energy computation for the FT quantization condition is harder to carry out analytically. For the numerical choice \( \alpha = 1, A = 2, B = 1 \), we see from Table 2 that the ground state energy \( E^{FT}_0 \) is lower than the exact energy by 3.2% whereas \( E^{WKB}_0 \) is higher than the exact energy by 9.7%.

5. Conclusion
We have given a complete analytic treatment of the energy levels of shape invariant potentials (with a translational change of parameters) for various semiclassical quantization conditions. As expected from previous work [7], the SWKB energy levels are exact. The WKB energy levels are exact for the one-dimensional harmonic oscillator and the Morse potentials only. For other potentials the results are not exact, and this has historically led to ad hoc Langer corrections [11]. Typically, one sees from Table 1 that the ground state energy from the WKB method deviates from the exact result by about 10%. The new semiclassical approach of Friedrich and Trost is exact only for the one-dimensional harmonic oscillator and no other shape invariant potential. However, in general, it gives significantly more accurate ground state energies than the WKB method.

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Table Captions

Table 1: List of all shape invariant potentials and their eigenvalues. Analytic expressions for the integrals in the WKB and SWKB quantization condition are given, along with the energy eigenvalues. For these potentials, the SWKB results are always exact, whereas the WKB results are exact only for the harmonic oscillator and Morse potentials.

Table 2: Comparison of the exact ground state energies of shape invariant potentials with results from the WKB and Friedrich-Trost method. The percent errors are also shown. The SWKB results are not shown, since they are always exact for the potentials under consideration.
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| Potential Type | Super Potential | Energy | WKB Minimum | Shape of Potential |
|---------------|----------------|--------|-------------|-------------------|
| Morse | $V_{	ext{Morse}}$ | $E$ | $E_w$ | Parabolic |
| Oscillator | $V_{	ext{Oscillator}}$ | $E$ | $E_w$ | Parabolic |

| Parameter | Expression |
|-----------|------------|
| $E_w$ | $E = \frac{1}{2}m\omega^2x^2 - V(0)$ |
| $V(0)$ | $V(0) = \frac{1}{2}kx^2$ |

Equations for the integrals in the WKB and SWKB quantization conditions are:

$$\int_{x_1}^{x_2} e^{-i\int dx} dx = \begin{cases} 1 & \text{if } x_1 < x_2 \\ 0 & \text{if } x_1 > x_2 \end{cases}$$

$$\int_{x_1}^{x_2} e^{i\int dx} dx = \begin{cases} 1 & \text{if } x_1 < x_2 \\ 0 & \text{if } x_1 > x_2 \end{cases}$$
| Name of Potential | Choice of Parameters | Super Potential | Potential $V(x)$ | $E_0^{exact}$ ($E_0^{exact}$) | $E_0^{WKB}$ | Percent error | Friedrich-Trost $E_0^{FT}$ | Percent error |
|-------------------|----------------------|-----------------|------------------|-----------------------------|--------------|---------------|-----------------------------|---------------|
| Shifted oscillator | —                    | $\frac{1}{2}\omega x$ | $\frac{1}{4}\omega^2 x^2$ | $\frac{\sqrt{2}}{\omega}$ | 2.1716 | 2 | 8.07% | 2.158 | 0.61% |
| Three dimensional oscillator | $\omega = 2$ | $l = 1$ | $r - \frac{2}{r}$ | $(\sqrt{2}/r - r)^2$ | 0.0625 | 0.5677 | 9.17% | 0.05580 | 10.7% |
| Coulomb | $e = 1$ | $l = 1$ | $\frac{1}{4} - \frac{2}{r}$ | $2(\frac{1}{r} - \frac{1}{4})^2$ | 3 | 3 | 0 | 2.7587 | 8.04% |
| Morse | $\alpha = 2$ | $A = 1$ | $1 - e^{-2x}$ | $(2 - e^{-2x})^2$ | 2.1030 | 9.72% | 1.8549 | 3.22% |
| Rosen-Morse II | $\alpha = 1$ | $A = 2$ | $2\tanh x + \frac{1}{2}$ | $\frac{1}{6}(1 + 6 \tanh x)^2$ | 1.9167 | 3 | 14.25% | 2.9356 | 2.14% |
| Eckart | $\alpha = 1$ | $A = 2$ | $3 - 2 \coth r$ | $2(\coth r - 3)^2$ | 7 | 6.511 | 7.00% | 6.1540 | 12.1% |
| Rosen-Morse I (trigonometric) | $\alpha = 1$ | $A = 2$ | $-1 - 2\cot x$ | $2(1 + \cot x)^2$ | 3 | 2.5727 | 14.25% | 2.9356 | 2.14% |
| Generalized Scarf II (hyperbolic) | $\alpha = 1$ | $A = 1$ | $\tanh x$ | $\frac{1}{\sqrt{10}} - \sqrt{10}$ | 1.0811 | 1.19257 | 10.31% | 1.02981 | 4.74% |
| Föschl-Teller | $\alpha = 1$ | $A = 1$ | $\coth r$ | $+11\text{csch}^2 r$ | 1.33772 | 1.2790 | 4.39% | 1.2576 | 5.99% |
| Scarf I (trigonometric) | $\alpha = 1$ | $A = 3$ | $3 \tan x$ | $+\frac{\sqrt{6}}{2} - \frac{\sqrt{6}}{2} - \sqrt{6}$ | 3.0505 | 2.689 | 11.8% | 3.1285 | 2.56% |

Table 2: Comparison of the exact ground state energies of shape invariant potentials with results from the WKB and Friedrich-Trost method. The percent errors are also shown. The SWKB results are not shown, since they are always exact for the potentials under consideration.