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New Quantization Method for Evaluation of Eigenenergies

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A quantum dynamical equation is constructed as the limit of a sequence of functions (called Semiquantum momentum functions or SQMF). The quantum action variable J is defined as the limit of the sequence of contour integrals of SQMFs such that the quantization condition is $J = n\hbar$, where n is a nonnegative integer for eigenvalues and a noninteger for off eigenvalues. This quantization condition is exact and J is an analytic function of energy. Based on new definitions, an accurate numerical method is developed for obtaining eigenenergies. The method can be applied to both real and PT symmetric complex potentials. The validity and the accuracy of this new method is demonstrated with three illustrations.

KEY WORDS: WKB; quantization; schroedinger equation; eigenenergies.

1. INTRODUCTION

During last few decades, various exact and approximation methods have been developed for solving 1-D quantum mechanical systems. They include Rayleigh–Schroedinger expansions summed by means of different techniques (Arteca *et al.*, 1990; Caliceti *et al.*, 1996; Fernández *et al.*, 1998; Simon, 1970), variational procedures (Bozzolo *et al.*, 1982), adjustable frequency iteration (Fanelli and Struzynski, 1983), distributed Gaussian basis (Balsa *et al.*, 1983), Laplace transform (Flessas *et al.*, 1983), strong coupling expansions (Guardiola *et al.*, 1992; Turbiner and Ushveridze, 1988), continued fractions (Znojil, 1983) related to the Hill determinant method (Hautot, 1986; Znojil, 1991), supersymmetry combined with variational (Cooper *et al.*, 1994) or WKB (Sinha *et al.*, 1996) techniques, analytical Lanczos algorithm (Kaluza, 1994), semiclassical expansions complemented with resurgence theory (Delabaere and Pham, 1997; Delabaere *et al.*, 1997), Kolmogorov iterative technique (Halperin, 1995), and open perturbation applied to the associated Riccati equation (Bessis and Bessis, 1997).

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The work which is relevant to this study is the method based on quantum action variable theory developed in 1980s by Leacock *et al.* (Leacock and Padgett, 1983a,b). Their method is mainly suitable for exactly solvable potentials for which the eigenenergies can be obtained without solving the dynamical equations (see (Leacock and Padgett, 1983a,b) for more details). Their method involves evaluating the 1-D quantum action variable (QAV) $J(E)$ defined as

$$J(E) = \int_{\mathrm{C}} p(z, E)\, dz \tag{1}$$

where the contour C encloses the physical turning points of classical momentum function $p_{\mathrm{c}}(z, E)$ in the complex z plane, and $p(z, E)$ is the quantum momentum function (QMF) which satisfies the equation

$$\frac{h}{i}\left(\frac{\partial p(z, E)}{\partial z}\right) + p^2(z, E) = p_{\mathrm{c}}^2(z, E) \tag{2}$$

where $p_{\mathrm{c}}(z, E)$ is defined by $p_{\mathrm{c}}(z, E) = \sqrt{E - V(z)}$ (assume $2m = 1$) and the boundstate boundary conditions imposed upon $p(z, E)$ is $p(z, E) \to p_{\mathrm{c}}(z, E)$ as $\hbar \to 0$. The bound state eigenvalue expressions of exactly solvable potentials can be obtained without solving the dynamical equation (Leacock and Padgett, 1983a,b; Nanayakkara, 1990). This method is somewhat similar to the higher order WKB (Bender *et al.*, 1977) method which also uses contour integrations for obtaining higher order corrections to the basic Bohr–Sommerfeld quantization (see (Bender *et al.*, 1977) for more details). There are two features of QAV method relevant to the present work:

(1) The quantum action variable $J(E)$ is not an analytic function of energy E (It is a step-function)
(2) The application of the boundary condition is not clear when the system is not exactly solvable

The QMF $p(z, E)$ is related to the wave function ψ by $p(z, E) = \frac{\hbar}{i}\frac{\partial\psi/\partial z}{\psi}$. Therefore, the contour integral (1) gives the number of simple zeros of ψ which are located between two turning points. By using oscillatory theorems on Sturm-Liouville type equations (Ince, 1927), it can be shown that there are a finite number of isolated zeros of $\psi(x)$ and hence finite number of isolated poles of $p(z, E)$, lying between two physical turning points for eigenvalues as well as for off eigenvalues. Hence, the QAV is an integer valued function which gives the number of zeros of the wave function between two physical turning points (see (Leacock and Padgett, 1983b)). As a result, when energy E varies, QAV jumps from one integer to the next as a new zero entered inside the contour C. Consequently, QAV is not an analytic function of E. The quantum action variable used in (Leacock and Padgett, 1983a,b; Nanayakkara, 1990) cannot be directly employed for locating bound state eigen states numerically when the system is not exactly solvable. The main reason for

this drawback is that $J(E)$ changes only when a new zero of ψ entered between two turning points which does not necessarily correspond to any special energy values such as eigenenergies.

In this paper, we reformulate quantum action variable theory in terms of sequence of newly defined functions (we call them semiquantum momentum functions – SQMF) and corresponding sequence of contour integrals (we call them semiquantum action variables – SQAV) such that they converge to QMF $p(z, E)$ and QAV $J(E)$, respectively, when certain conditions are satisfied by the potential. With this new approach, we developed an accurate numerical method. This new method is applied to solve three potentials including PT symmetric complex potential $v(x) = x^4 + iAx$ (Bender *et al.*, 2001).

The outline of the paper is as follows. In Section 2, the basic theory is developed with proper quantization conditions. Section 3 contains explicit algebraic form of new SQMFs and a description of the numerical method. Also we discuss the convergence and the validity of the new method. In Section 4 the accuracy of the numerical method is demonstrated with three illustrations.

2. QUANTUM ACTION VARIABLE THEORY

For 1-D quantum mechanical system with potential $v(z)$, a sequence of functions $\{p_k(z, E)\}$, $k = 1, 2, 3, \ldots n$, is defined in the complex z plane by

$$p_0(z, E) = \sqrt{E - v(z)}, \tag{3}$$

$$p_n(z, E) = \sqrt{E - v(z) + i\hbar \frac{\partial p_{n-1}}{\partial z}}, \tag{4}$$

where $p_0(z, E)$ is the usual classical momentum function, and the Eq. (4) defines $p_n(z, E)$ in terms of the first derivative of $p_{n-1}(z, E)$. Hence starting from Eq. (3), the Eq. (4) can be used iteratively to define $p_k(z, E)$ for any k. Here we have assumed $2m = 1$. We call these functions "semiquantum momentum functions" rather than semiclassical momentum function, in order to distinguish them from WKB momentum (see Appendix A). When certain conditions are satisfied by the potential, $p_k(z, E)$ converges uniformly as $k \to \infty$ in the domain $D(E)$, which is shown in Fig. 1, when $\hbar$ is less than unity. This will be discussed in detail in the Appendix A.

Let $\tilde{p}(z, E)$ be the limit of the sequence. That is

$$\tilde{p}(z, E) = \lim_{n\to\infty} p_n(z, E) \quad \forall x \in D(E) \tag{5}$$

For different energies, domain $D(E)$ may change, as the turning points of $p_k(z, E)$ are functions of energy. However, for a given range of energies, a single $D(E)$ can be defined such that it excludes turning points corresponding to all the energies in the range and hence the limit in Eq. (5) exists for a range of energy values.

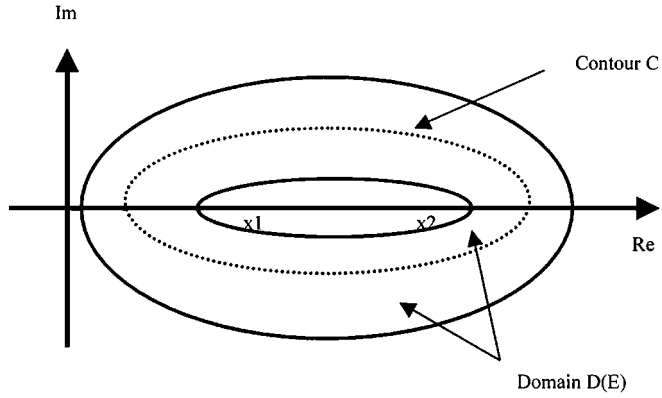

Fig. 1. The complex plane on which the SQMF, SQAVs, and QAV are defined. It can be shown that SQMF converges uniformly in the domain $D(E)$. The contour C in Eqs. (7) and (8) is shown as a broken curve in the domain $D(E)$.

Consequently, the sequence $\{p_k(z, E)\}$, $k = 1, 2, 3, \ldots n$ converges uniformly not only in x but also in E.

The limiting function $\tilde{p}(z, E)$ is defined to be the new quantum momentum function satisfying the equation

$$\tilde{p}(z, E) = \sqrt{E - v(z) + i\hbar \frac{\partial \tilde{p}}{\partial z}} \tag{6}$$

Although the $p_k(z, E)$ converges uniformly to $\tilde{p}(z, E)$ only in the domain $D(E)$, $\tilde{p}(z, E)$ can be analytically continued to the entire complex plane by defining it with the Eq. (6) for all z.

Now we define semiquantum action variables (SQAV) $J_k(E)$, $k = 1, 2, 3, \ldots n$, as

$$J_k(E) = \frac{1}{2\pi} \int_C p_k(z, E)\, dz \tag{7}$$

where the contour C encloses the "physical" turning points of the first k SQMFs and lies entirely in the domain $D(E)$ (see Fig. 1). Since $p_k(z, E)$ is uniformly convergent, $J_k(E)$ is also uniformly convergent, $\lim_{k\to\infty} J_k(E) = \tilde{J}(E)$, and the limit $\tilde{J}(E)$ satisfies the equation

$$\tilde{J}(E) = \frac{1}{2\pi} \int_C \tilde{p}(z, E)\, dz \tag{8}$$

where $\tilde{p}(z, E)$ satisfies Eq. (6) and the contour encloses the "physical" turning points of $\{p_k(z, E)\}$, $k = 1, 2, 3, \ldots n$. Now we introduce the quantization condition imposed upon $\tilde{J}(E)$ as

$$\tilde{J}(E) = n\hbar \tag{9}$$

where n is a nonnegative integer.

Note that by squaring both sides of Eq. (6) and rearranging it, we obtain

$$\frac{\hbar}{i}\frac{\partial \tilde{p}}{\partial z} + \tilde{p}^2(z, E) = E - v(z) \tag{10}$$

which is equivalent to the Eq. (2), although $\tilde{p}(z, E)$ is not identical to $p(z, E)$. Identification of following features of new QMF $\tilde{p}(z, E)$ and QAV $\tilde{J}(E)$ is useful.

(a) The new QMF is a multivalued function of x unlike the old QMF which is single valued.
(b) The new QAV is a nonnegative integer times $\hbar$ for eigenvalues and non-integer times $\hbar$ for off eigenvalues and it is analytic function of E. The old QAV is an integer times $\hbar$ for all energies and it is discontinuous at certain energies.

These features are utilized when the numerical methods are developed.

3. ANALYTIC FORM OF SQMF

The algebraic form of $p_0(z, E)$ is given by Eq. (3);

$$p_0(z, E) = \sqrt{E - v(z)}$$

Starting with Eq. (3) and using Eq. (4) iteratively, we obtain

$$p_1(z, E) = \sqrt{E - v(z) - i\hbar\frac{v'(z)}{2p_0}} \tag{11}$$

$$p_2(z, E) = \sqrt{E - v(z) + i\hbar\,\frac{\partial p_1}{\partial z}} \quad \text{with} \quad \frac{\partial p_1}{\partial z} = -\left(\frac{v'}{2p_1} + \frac{i\hbar v'^2}{8p_0^3 p_1} + \frac{i\hbar v''}{4p_0 p_1}\right). \tag{12}$$

With mathematical packages such as Mathematica (Wolfram, 1988), it is easy to obtain exact algebraic expressions up to any order of SQAV.

Now we are going to describe how to use new definitions to obtain eigenvalues for a given quantum system. When the orders of p_k is four or above (i.e. $k \geq 4$), it is hard to implement the algebraic expressions of $p_k(x, E)$ directly into a computer code. The reason for this difficulty is that the expressions become so huge and complicated that there is no easy way of breaking them (specially the square roots) into simpler expressions. However, the recurrence relations of p_k (in Eq (4)) can easily be implemented by writing them in terms of new functions $\xi_k(\eta)$ and $\eta_k(x, E)$, $k = 0, 1, \ldots n$, which are suitable for computer implementations. The new $\xi_k(\eta)$ and $\eta_k(x, E)$ are functions of $p_0(x, E)$ and the derivatives of the potential. The explicit forms of ξ_0, ξ_1, ξ_2, ξ_3, ξ_4, and ξ_5 are given in Appendix B.

The algebraic expressions of the quantum momentum function along with the derivatives of $\eta_k(x, E)$'s are given below. The zeroth order SQMF can be written as

$$p_0 = \sqrt{\eta_0} \tag{13}$$

where $\eta_0 = p_0^2 = E - v(x)$. The derivatives of η_0 can be written in terms of the derivative of the potential

$$\frac{\partial^k \eta_0(x, E)}{\partial x^k} = -\frac{d^k v(x)}{d^k x} \quad k = 1, 2, \ldots n \tag{14}$$

where $v(x)$ is the potential. The rth order SQMF $p_r(x, E)$ is given by

$$p_r = \sqrt{\eta_r} \tag{15}$$

where $\eta_r = \eta_0 + i\hbar\xi_1(\eta_{r-1})$ and the derivatives of η_r are

$$\frac{\partial^k \eta_r(x, E)}{\partial x^k} = \frac{\partial^k \eta_0(x, E)}{\partial x^k} + i\hbar\xi_{k+1}(\eta_{r-1}) \tag{16}$$

where $\xi_r(\eta) = \frac{\partial^r \sqrt{\eta}}{\partial x^r}$ and explicit forms of $\xi_k(\eta)$ for $k = 1, 2, \ldots 6$ are given in Appendix B.

Using Eqs. (13), (14), (15), and (16), one can write the SQMFs up to any order in terms of the classical momentum function and the derivatives of the potential. Note that the first n derivatives of η_0 are needed to write the nth order SQMF. Note also that in evaluating the semiquantum momentum functions, the derivatives of η or $\xi_k(\eta)$ are calculated analytically, not numerically.

4. ILLUSTRATIONS: BOUND STATE ENERGIES

In this section, we present results obtained by applying the new quantization method described in the previous section to three different type of potentials.

(a) Potential $v(x) = x^2 + \frac{a^2}{x^2}$ with $a^2 = 0.1$.

This system is exactly solvable (Nanayakkara, 1990) and the quantum action variable is

$$J = \frac{E}{4} - \frac{\hbar}{2} - \frac{\sqrt{a^2 + \frac{\hbar^2}{4}}}{2} \tag{17}$$

For this potential there are four real turning points, two of them on the positive real axis while the other two are on the negative real axis. Here we have the freedom to choose any contour enclosing two turning points on the positive real axis which excludes the origin ($x = 0$) where the potential has a singularity. This system is studied with 7th order SQMF and the contour integration is evaluated with a rectangular contour. The results are presented in the Table I. The table shows that the error is less than 10^{-10} for a 7th order calculation.

Table I. Comparison Between the Exact and the Calculated Boundstate Energies of the Potential $v(x) = x^2 + \frac{a^2}{x^2}$ ($\hbar = 0.001$ and $a^2 = 0.1$)

n	Exact energy	Calculated energy	Error
0	0.6344563226025	0.6344563226025	$<10^{-11}$
1	0.6384563226025	0.6384563226025	$<10^{-11}$
2	0.6424563226025	0.6424563226025	$<10^{-11}$
3	0.6464563226025	0.6464563226025	$<10^{-11}$
4	0.6504563226025	0.6504563226025	$<10^{-11}$
5	0.6544563226025	0.6544563226026	$\approx 10^{-10}$
6	0.6584563226025	0.6584563226026	$\approx 10^{-10}$
7	0.6624563226025	0.6624563226026	$\approx 10^{-10}$
8	0.6664563226025	0.6664563226026	$\approx 10^{-10}$
9	0.6704563226025	0.6704563226026	$\approx 10^{-10}$
10	0.6744563226025	0.6744563226026	$\approx 10^{-10}$

Note that in this numerical method, SQMF has to be evaluated only at the points of the contour and therefore it is computationally less expensive.

(b) Potential $v(x) = x^4 + bx^2$.

This system cannot be solved exactly. For this potential, there are four turning points: two of them are on the real axis and the other two are on the imaginary axis.

$$\pm\left[\frac{-b+\sqrt{b^2+4E}}{2}\right]^{1/2} \quad \text{and} \quad \pm i\left[\frac{b+\sqrt{b^2+4E}}{2}\right]^{1/2}$$

Here we choose a contour of integration to enclose two real turning points and to exclude the turning points on the imaginary axis. In this region the sequences p_n and J_n converges rapidly. The results of the calculations carried out with 7th order SQMF for this potential are presented in the Tables II and III.

The calculations were carried out for two values of the coupling parameter b. The exact eigenenergies of this potential were obtained by expanding the wave function in simple harmonic basis and solving the corresponding matrix eigenvalue problem. As shown in the Tables II and III, the accuracy of the calculation increases with the quantum number n. This asymptotic behavior can be expected as this new method is closely related to the WKB method (see Appendix A). With this new method we were able to obtained eigenenergies with very few iterations.

(c) Potential $v(x) = x^4 + iAx$.

The last illustration is the PT symmetric complex potential $v(x) = x^4 + iAx$. There have been great interest in PT symmetric complex potentials with real positive energy spectra as it was found that quantum field theories analogous to the quantum mechanical theory for them have

Table II. Comparison Between the Exact Numerical Values and the Calculated Values for $v(x) = x^4 + 0.1x^2$ ($\hbar = 0.01$)

n	Exact	Calculated	Error
0	0.0037029004	0.003710245	−0.001983472
1	0.01189426805	0.0118957944	−0.000128327
2	0.02140481142	0.0214050053	−9.05778E-06
3	0.0318761422	0.0318762039	−1.93562E-06
4	0.0431371927	0.0431372167	−5.56364E-07
5	0.055079058	0.0550790694	−2.06975E-07
10	0.122853411	0.1228534114	−3.25591E-09
20	0.287168691	0.2871686914	−1.39291E-09
30	0.478767632	0.4787676320	0
40	0.691271268	0.6912712677	4.33983E-10
50	0.921110458	0.9211104577	3.25694E-10
100	2.266962730	2.266962729	4.41119E-10

amazing properties (Bender *et al.*, 2001). For small values of A, all energy levels are real and positive. However, if A increases beyond threshold values, adjacent pairs of energy levels coalesce and then become complex (Bender *et al.*, 2001). In order to solve Schroedinger equation for this potential, one has to carry out the integration not along the real axis but along anti-Stokes lines (Bender *et al.*, 2001). However, in this study we found that the numerical method introduced in this paper is very suitable for solving such systems with less complications.

For this potential, there are four turning points, all of them are complex (see Fig. 2). We evaluated the contour integral with a rectangular contour enclosing two lower turning points as shown in Fig. 2. When

Table III. Comparison Between the Exact Numerical Values and the Calculated Values for $v(x) = x^4 + 10x^2$ ($\hbar = 0.01$)

n	Exact	Calculated	Error
0	0.031630272	0.0316302701	6.0069E-08
1	0.0949057972	0.0949057949	2.42346E-08
2	0.158211261	0.1582112595	9.48099E-09
3	0.221546625	0.2215466237	5.86784E-09
4	0.284911849	0.2849118476	4.9138E-09
5	0.348306893	0.3483068916	4.01944E-09
10	0.665728031	0.6657280297	1.95275E-09
20	1.302784329	1.3027843275	1.15138E-09
30	1.942760925	1.9427609238	6.17678E-10
40	2.585620837	2.5856208356	5.41456E-10
50	3.231328273	3.2313282714	4.95152E-10
100	6.501401680	6.5014016789	1.69194E-10

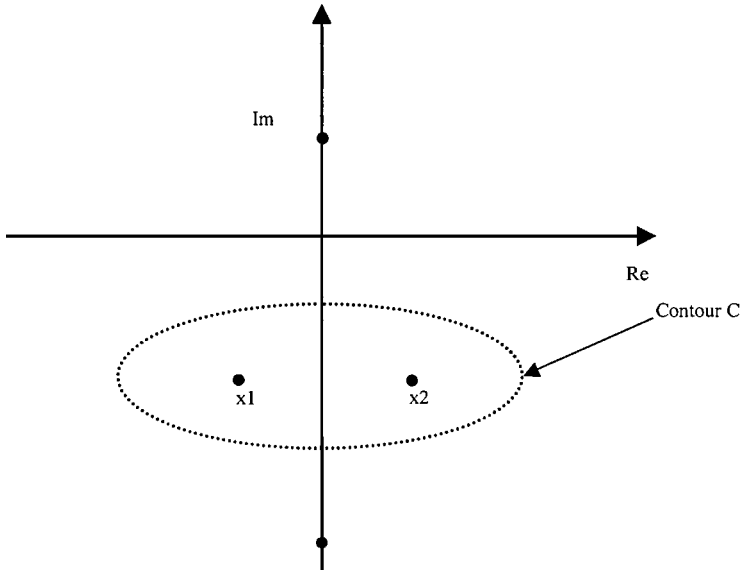

Fig. 2. The four complex turning points for the potential $v(x) = x^4 + iAx$ are shown. The contour encloses only the middle two turning points marked with solid circle (•). The other two turning points which are on the imaginary axis are kept outside the contour of integration.

the contour was kept away from turning points which are located above and below, this method produced accurate real positive eigenvalues. However, for the first two eigenvalues, this method did not converge. As for the previous potential, the accuracy of the calculation increased with higher excited states. The results are shown in Table IV.

Table IV. Comparison Between the Exact Numerical Values and the Calculated Values for $v(x) = x^4 + iAx$ ($\hbar = 0.01$)

n	Exact	Calculated	Error
2	0.0165265275	0.0164755069	0.003087194
3	0.0254315237	0.0254341551	0.00010347
4	0.0353335816	0.0353334087	4.89336E-06
5	0.0460201330	0.0460201279	1.10821E-07
10	0.1084473067	0.1084473048	1.752E-08
20	0.2642551559	0.2642551538	7.94686E-09
30	0.4487085662	0.4487085638	5.34868E-09
40	0.6548295643	0.6548295617	3.9705E-09
50	0.8787998557	0.8787998492	7.39645E-09
100	2.1996949309	2.199694923	3.59141E-09

5. DISCUSSION

In this paper we presented a new quantization method for 1-D systems. The semiquantum momentum function, defined in this paper links classical mechanics with quantum mechanics in 1-D, systematically, starting from p_0 being classical momentum function to $\lim_{n\to\infty} p_n$ being purely a quantum mechanical quantity which is directly related to the quantum wave function. With three illustrations, we demonstrated the validity and the applicability of the method for various types of potentials. Although we have not given a rigorous proof for the convergence of the method, discussion given in Appendix A and the illustrations show how to choose contours on which p_n and J_n are convergent.

APPENDIX A

In this appendix we discuss the convergence of the sequence of SQMF p_n and SQAV J_n. First we compare the SQMF with usual WKB expansion. This is useful when we discuss the convergence later in this section.

Since the expansion of any order (>0) of SQMF contain all the powers of $\hbar$, nth order SQMF is not the same as the nth order WKB. However, they are related in an interesting manner. The usual WKB expansion of potential $v(x)$ is

$$\tilde{p}(x, E) = \tilde{p}_0 + \hbar\tilde{p}_1 + \hbar^2\tilde{p}_2 + \cdots \hbar^n\tilde{p}_n + \cdots \tag{A1}$$

Please note that $\tilde{p}(x, E)$ here corresponds to the derivative of the action in the usual WKB ansatz, where

$$\tilde{p}_0 = \sqrt{E - v(x)},$$

$$\tilde{p}_1 = \frac{-iv'}{4(E-v)},$$

$$\tilde{p}_2 = \frac{(5v'^2 + 4Ev'' - 4vv'')}{32(E-v)^{5/2}},$$

$$\tilde{p}_3 = \frac{15iv'^3}{64(E-v)^4} + \frac{9iv'v''}{(E-v)^3} + \frac{iv'''}{16(E-v)^2},$$

$$\tilde{p}_4 = -\left\{\frac{1105v'^4}{2048(E-v)^{11/2}} + \frac{221v'^2v''}{256(E-v)^{9/2}} + \frac{19v''^2}{128(E-v)^{7/2}} + \frac{7v'v'''}{32(E-v)^{7/2}} + \frac{9v^{(4)}}{32(E-v)^{5/2}}\right\}$$

(where $v^{(4)}$ is the forth derivative of v with respect to x) and so on. Here we have given the first five terms in the WKB expansion explicitly. Now we expand the

first five terms of the SQMF in powers of $\hbar$.

$$
\begin{aligned}
p_0 &= \sqrt{E - v(x)},\\
p_1 &= \sqrt{E - v(x)} - \frac{iv'\hbar}{4(E-v)} + \frac{v'^2\hbar^2}{32(E-v)^{5/2}} + \frac{iv^{(3)}\hbar^3}{128(E-v)^4}\\
&\quad - \frac{5v^{(4)}\hbar^4}{2048(E-v)^{11/2}} + O(\hbar^5),\\
p_2 &= \sqrt{E - v(x)} - \frac{iv'\hbar}{4(E-v)} + \frac{(5v'^2 + 4Ev'' - 4vv'')\hbar^2}{32(E-v)^{5/2}}\\
&\quad + \left[\frac{5iv^{(3)}}{64(E-v)^4} + \frac{iv'v''}{16(E-v)^3}\right]\hbar^3 - \left[\frac{97v'^4}{2048(E-v)^{11/2}}\right.\\
&\quad \left. + \frac{3v'^2v''}{64(E-v)^{9/2}} + \frac{v''^2}{128(E-v)^{7/2}}\right]\hbar^4 + O(\hbar^5),\\
p_3 &= \sqrt{E - v(x)} - \frac{iv'\hbar}{4(E-v)} + \frac{(5v'^2 + 4Ev'' - 4vv'')\hbar^2}{32(E-v)^{5/2}}\\
&\quad + \frac{15iv'^3\hbar^3}{64(E-v)^4} + \frac{9iv'v''\hbar^3}{32(E-v)^3} + \frac{iv^{(3)}\hbar^3}{16(E-v)^2}\\
&\quad - \frac{465v'^4\hbar^4}{2048(E-v)^{11/2}} - \frac{77v'^2v''\hbar^4}{256(E-v)^{9/2}} - \frac{5v''^2\hbar^4}{128(E-v)^{7/2}}\\
&\quad - \frac{3v'v^{(3)}\hbar^4}{64(E-v)^{7/2}} + O(\hbar^5),
\end{aligned}
$$

and

$$
\begin{aligned}
p_4 &= \sqrt{E - v(x)} - \frac{iv'\hbar}{4(E-v)} + \frac{(5v'^2 + 4Ev'' - 4vv'')\hbar^2}{32(E-v)^{5/2}} + \frac{15iv'^3\hbar^3}{64(E-v)^4}\\
&\quad + \frac{9iv'v''\hbar^3}{32(E-v)^3} + \frac{iv^{(3)}\hbar^3}{16(E-v)^2} - \frac{1105v'^4\hbar^4}{2048(E-v)^{11/2}} - \frac{221v'^2v''\hbar^4}{256(E-v)^{9/2}}\\
&\quad - \frac{19v''^2\hbar^4}{128(E-v)^{7/2}} - \frac{7v'v^{(3)}\hbar^4}{32(E-v)^{7/2}} - \frac{v^{(4)}\hbar^4}{32(E-v)^{5/2}} + O(\hbar^5).
\end{aligned}
$$

By comparing expressions of SQMF with the WKB expansion, the following observations can be made.

The first n coefficients of p_n are the same as first n coefficients of the WKB expansion. That is, if $a_{n,m}$ is the coefficient of the $\hbar^m$ term in the nth order SQMF, then $a_{n,m} = m$th order WKB term for $\forall m < n$. In other words, *the expansion of*

nth order SQMFs contain all the terms of nth order WKB expansion, in addition to the terms of higher powers of $\hbar$. By using this observation, we propose the following result.

When $\hbar < 1$, the sequence of SQMFs $\{p_k, k = 0, 1, 2, \ldots n\}$ converges uniformly in a domain where $|\frac{i\hbar\partial p_k/\partial x}{p_0^2}| < 1$ for $k = 0, 1, 2, \ldots n$. The simple proof for this result can be given. The above condition implies that $p_n(x)$ can be expanded in a power series of $\hbar$.

$$p(x, E) = p_0 + \hbar a_1 + \hbar^2 a_2 + \cdots \hbar^n a_n + \cdots$$

where

$$a_n = -\left[\frac{i\,\partial p_{n-1}/\partial x}{p_0^2}\right] b_n \quad b_n = \frac{1.3 \ldots (2n-5)}{2.4.6 \ldots 2(n-1)}$$

Now consider the WKB expansion (18). Let S_n, be the nth partial sum of the above series. Previously in this appendix we concluded that the first n terms of the expression for p_n is the same as the nth partial sum of the WKB expansion. Hence

$$[p_n - S_n] = -\left[\frac{i\hbar\partial p_k/\partial x}{p_0^2}\right]^{n+1} b_{n+1} - \left[\frac{i\hbar\partial p_k/\partial x}{p_0^2}\right]^{n+2} b_{n+2} - \cdots$$

Therefore $\lim[p_n - S_n] = 0$ as $n \to \infty$ and consequently $\lim p_n = \lim S_n$. Since WKB partial sums S_n converges uniformly to $\tilde{p}$ when x is not near turning points, p_n converges to $\tilde{p}$ as well.

APPENDIX B

In this appendix we express the functions $\xi(\eta)$ in terms of the derivatives of η. The functions $\xi(\eta)$ are defined as $\xi_r(\eta) \equiv \frac{\partial^r \sqrt{\eta}}{\partial x^r}$. The functions $\xi_n(\eta)$ for $n = 1, 2, \ldots 6$ are given below.

$$\xi_1(\eta) = \frac{\eta'(x)}{2\sqrt{\eta(x)}}$$

$$\xi_2(\eta) = \frac{-\eta'(x)^2}{4\eta(x)^{3/2}} + \frac{\eta''(x)}{2\sqrt{\eta(x)}}$$

$$\xi_3(\eta) = \frac{3\eta'(x)^3}{8\eta(x)^{5/2}} - \frac{3\eta'(x)\eta''(x)}{4\eta(x)^{3/2}} + \frac{\eta^{(3)}(x)}{2\sqrt{\eta(x)}}$$

$$\xi_4(\eta) = \frac{-15\eta'(x)^4}{16\eta(x)^{7/2}} + \frac{9\eta'(x)^2\eta''(x)}{4\eta(x)^{5/2}} - \frac{3\eta''(x)^2}{4\eta(x)^{3/2}} - \frac{\eta'(x)\eta^{(3)}(x)}{\eta(x)^{3/2}} + \frac{\eta^{(4)}(x)}{2\sqrt{\eta(x)}}$$

$$\xi_5(\eta) = \frac{105\eta'(x)^5}{32\eta(x)^{9/2}} - \frac{75\eta'(x)^3\eta''(x)}{8\eta(x)^{7/2}} + \frac{45\eta'(x)\eta''(x)^2}{8\eta(x)^{5/2}} + \frac{15\eta'(x)^2\eta^{(3)}(x)}{4\eta(x)^{5/2}} - \frac{5\eta''(x)\eta^{(3)}(x)}{2\eta(x)^{3/2}} - \frac{5\eta'(x)\eta^{(4)}(x)}{4\eta(x)^{3/2}} + \frac{\eta^{(5)}(x)}{2\sqrt{\eta(x)}}$$

$$\xi_6(\eta) = \frac{-945\eta'(x)^6}{64\eta(x)^{11/2}} + \frac{1575\eta'(x)^4\eta''(x)}{32\eta(x)^{9/2}} - \frac{675\eta'(x)^2\eta''(x)^2}{16\eta(x)^{7/2}} + \frac{45\eta''(x)^3}{8\eta(x)^{5/2}} - \frac{75\eta'(x)^3\eta^{(3)}(x)}{4\eta(x)^{7/2}} - \frac{45\eta'(x)\eta''(x)\eta^{(3)}(x)}{2\eta(x)^{5/2}} - \frac{5\eta^{(3)}(x)^2}{2\eta(x)^{3/2}} + \frac{45\eta'(x)^2\eta^{(4)}(x)}{8\eta(x)^{5/2}} - \frac{15\eta''(x)\eta^{(4)}(x)}{4\eta(x)^{3/2}} - \frac{3\eta'(x)\eta^{(5)}(x)}{2\eta(x)^{3/2}} + \frac{\eta^{(6)}(x)}{2\sqrt{\eta(x)}}$$

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