WKB and MAF quantisation rules for spatially confined quantum mechanical systems

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Abstract

A formalism is developed to obtain the energy eigenvalues of spatially confined quantum mechanical systems in the framework of the usual Wentzel-Kramers-Brillouin (WKB) and Modified Airy Function (MAF) methods. To illustrate the working rule, the techniques are applied to 3 different cases, viz. the confined 1-dimensional harmonic and quartic oscillators, and a boxed-in charged particle subject to an external electric field. The energies thus obtained are compared with those from shifted 1/N expansion, variational and other methods, as well as the available exact numerical results.

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I Introduction

Spatially confined quantum mechanical systems [1-3] make an interesting study due to their importance in a variety of physical problems - e.g. studying thermodynamic properties of non-ideal gases, investigation of anharmonic effects in solids, in atoms and in molecules under high pressure, impurity binding energies in quantum wells and near-surface donor states, and even in the context of partially ionised plasmas. When an atom or a molecule is trapped inside any kind of microscopic cavity, it suffers a spatial confinement that affects its physical and chemical properties [1,2,4]. The same situation occurs for mesoscopic scale semiconductor artificial structures like 2-dim. quantum wells [5-7], quantum-well wires [8,9] and quantum dots [10-14], where impurity or excitonic states are influenced by the small sizes of these structures. Spatial confinement, also called the boxing effect, significantly influences the bond formation and chemical reactivity inside the cavities [1,2,4]. There are many natural or artificial cavities that could produce sensitive effects — zeolite molecular sieves, fullerenes, or even mono-or 2-dimensional cavities formed by large organic molecules [1, 2].

An infinite barrier model is the one most commonly used to study the problems on spatial confinement. In order to know the energy eigenvalues and eigenfunctions of such systems, one has to solve the corresponding Schrödinger equation. However, only a few potentials are exactly solvable; more so, the number of exactly solvable confined quantum mechanical potentials is extremely limited. Consequently, one has to apply various approximation techniques like the direct variational method [3,15], the shifted $1/N$ expansion procedure [12,16] etc. or do the same numerically. It would therefore be useful to develop formalisms which could study the different interpretations of the effects of the spatial confinement, in the framework of both solvable and unsolvable potentials analytically. The recent article by Krähmer et. al. [17] gives an outstanding historical account of confined quantum systems together with the theoretical methods for treating them. It gives perspective on the different confinement models: hard boxes and soft boxes, hypervirial theorem approaches etc.

With this goal in mind, we shall develop in this paper, a formalism for studying such spatially confined quantum mechanical systems in the framework of (usual) WKB (Wentzel-Kramers-Brillouin) and MAF (Modified Airy Function) methods. The WKB approxima-
tion results in a modified Bohr-Sommerfeld quantization rule in this context. To test the reliability of our formalisms, we shall apply our technique to 3 cases —

1. Confined 1-dimensional harmonic oscillator (HO), which is one of the most extensively studied model, both in classical as well as in quantum mechanics, due to its simplicity and usefulness. It is extremely important for the quantum mechanical treatment of problems involving vibrations of individual atoms in molecules and crystals [18]. Even the vibrations of the electromagnetic field in a cavity can be analysed into harmonic normal modes, each of which has energy levels of the oscillator type. Moreover, in the study of 2-dimensional and 3-dimensional quantum dots [10], the isotropic parabolic potentials are taken to be of the harmonic oscillator type

\[ V(\rho) = \frac{1}{4} \gamma^2 \rho^2 \quad \text{and} \quad V(r) = \frac{1}{4} \gamma^2 r^2 \]

respectively.

2. The 1-dimensional confined quartic oscillator (QO), which is of practical interest in molecular physics and in quantum field theory [15,19].

3. The interesting problem of a charged particle in an isolated quantum well structure, subject to an external electric field F [20].

The most widely studied confined systems are the harmonic and anharmonic oscillators, [2,15,20] and the hydrogen atom [3]. It is worth mentioning here that Vawter [21] employed the WKB method to study the confined one-dimensional harmonic oscillator, and obtained pretty accurate eigenvalues. Krähmer et. al. [17] investigated the parabolically confined Hydrogen atom in the WKB approximation and obtained a modified Bohr-Sommerfeld quantization rule, giving pretty accurate energy eigenvalues. However, we shall apply our formalism to nonsolvable potentials as well, viz, the boxed-in quartic oscillator and a charged particle in a box subject to an external electric field. Recently, a matrix formulation of the Bohr-Sommerfeld quantisation rule was applied to study bound states in 1-dimensional quantum wells [20]. Though our results agree with theirs in case of the 1-dimensional harmonic and quartic oscillators, it seems that their analytical result given for a confined charged particle under the influence of an external electric field F, is not compatible with what one would expect for large values of the confinement parameter. Very recently, Spehner et. al. [22] have applied the WKB method to a similar but more
complex quantum system, viz. non-interacting electrons constrained to a 2-dimensional domain with boundaries in the presence of a uniform perpendicular magnetic field.

The organisation of the paper is as follows. In section II we develop a formalism for the WKB quantisation rule for confined quantum mechanical systems. In section III we give the MAF formalism for the same. Section IV is kept for discussions and conclusions.

II WKB formalism for confined systems

The WKB (Wentzel-Kramers-Brillouin) approximation technique has been extremely useful in estimating the eigenfunctions and eigenvalues of the Schrödinger equation (yielding exact values for the harmonic oscillator). Our attempt here is to develop a formalism for studying spatially confined quantum mechanical systems in the framework of usual WKB quantisation rule, imposing appropriate boundary conditions. Though this method has been employed by others to solve confined systems, viz. parabolically confined hydrogen atom [17], 1-d harmonic oscillator [21], and non-interacting electrons in a uniform magnetic field constrained to a 2-dimensional domain with boundaries [22], our approach is different and works for other potentials as well.

We start with the 1-dimensional Schrödinger equation

$$\left\{ \frac{d^2}{dx^2} + \Gamma^2(x) \right\} \psi(x) = 0$$

(1)

where

$$\Gamma^2(x) = \frac{2m}{\hbar^2} \{ E - V(x) \}$$

(2)

We shall work in units

$$\hbar = c = 2m = 1$$

We take the confining potential to be such that it exists only in the region $-b < x < b$, and is infinite elsewhere.

$$V(x) = V(x) \quad \text{for} \quad -b < x < b$$

$$\infty \quad \text{for} \quad |x| > b$$

(3)

This imposes the boundary condition
\[ \psi(x = \pm b) = 0 \]  

We shall deal with symmetric profiles only, so that

\[ \Gamma^2(x) = \Gamma^2(-x) \]  

and the eigenfunctions are either symmetric or antisymmetric in \( x \). Hence

\[
\begin{align*}
\psi(0) &= 0 \quad \text{for the antisy} \\
\psi'(0) &= 0 \quad \text{for the symmetric function}
\end{align*}
\]  

Let \( x_t \) denote the turning point (where \( \Gamma^2(x) = 0 \))

**a) Turning point inside the box \( (x_t < b) \)**

Considering only the half space \( 0 < x < \infty \), the WKB solution in region I is

\[ \psi_I(x) = \frac{a_1}{\sqrt{\Gamma(x)}} \sin \left( \int_0^x \Gamma(x) dx \right) + \frac{a_2}{\sqrt{\Gamma(x)}} \cos \left( \int_0^x \Gamma(x) dx \right) \]  

Now \( \int_0^x \Gamma(x) dx \) can be written as

\[ \int_0^x \Gamma(x) dx = \int_0^{x_t} \Gamma(x) dx - \int_x^{x_t} \Gamma(x) dx = \alpha - \left( \theta_x + \frac{\pi}{4} \right) \]  

where

\[ \alpha = \int_0^{x_t} \Gamma(x) dx + \frac{\pi}{2} \]  

\[ \theta_x = \int_x^{x_t} \Gamma(x) dx \]  

Then \( \psi_I(x) \) can be written as

\[
\begin{align*}
\psi_I(x) &= \frac{1}{\sqrt{\Gamma(x)}} \left( a_1 \sin \alpha + a_2 \cos \alpha \right) \cos \left( \theta_x + \frac{\pi}{4} \right) \\
&\quad + \frac{1}{\sqrt{\Gamma(x)}} \left( a_2 \sin \alpha - a_1 \cos \alpha \right) \sin \left( \theta_x + \frac{\pi}{4} \right)
\end{align*}
\]
Making use of the connection formulae for WKB approximation [23]

\[
\frac{2}{\sqrt{\Gamma(x)}} \sin \left( \int_x^{x_t} \Gamma(x) dx + \pi/4 \right) \equiv \frac{1}{\sqrt{\kappa(x)}} \exp \left( - \int_{x_t}^x \kappa(x) dx \right) \quad (12)
\]

\[
\frac{1}{\sqrt{\Gamma(x)}} \cos \left( \int_x^{x_t} \Gamma(x) dx + \pi/4 \right) \equiv \frac{1}{\sqrt{k(x)}} \exp \left( + \int_{x_t}^x \kappa(x) dx \right) \quad (13)
\]

where

\[
\kappa^2(x) = -\Gamma^2(x) \quad (14)
\]

the wave function in region II can be written as

\[
\psi_{II}(x) = \left( a_1 \sin \alpha + a_2 \cos \alpha \right) \frac{1}{\sqrt{\kappa(x)}} \exp \left( \int_{x_t}^x \kappa(x) dx \right) + \left( a_2 \sin \alpha - a_1 \cos \alpha \right) \frac{1}{2\sqrt{k(x)}} \exp \left( - \int_{x_t}^x \kappa(x) dx \right) \quad (15)
\]

(i) For the antisymmetric function, the boundary condition (6) gives

\[
\psi_I(0) = 0
\]

so that from (7),

\[
a_2 = 0 \quad (16)
\]

Hence the confinement condition (4) (viz. \(\psi_{II}(b) = 0\)) gives

\[
e^{\beta} \sin \alpha - \frac{1}{2} e^{-\beta} \cos \alpha = 0 \quad (17)
\]

(ii) For the symmetric eigenfunction,

\[
\psi'_I(0) = 0
\]

so that

\[
a_1 = 0 \quad (18)
\]

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Hence the confinement condition (4) gives

\[ e^\beta \cos \alpha + \frac{1}{2} e^{-\beta} \sin \alpha = 0 \]  

(19)

In (17) and (19), \( \beta \) stands for

\[ \beta = \int_{x_t}^{b} \kappa(x)dx \]  

(20)

Thus the usual asymptotic WKB quantisation rule gets modified for spatially confined 1-dimensional quantum mechanical systems, and is given by eqns. (17) and (19) for the antisymmetric and symmetric wave functions respectively, provided the turning point is inside the confining box; i.e. \( x_t < b \).

b) Turning point outside the box \( (x_t > b) \)

However, for \( x_t > b \), i.e. in case the turning point lies beyond the confining length \( b \), the boundary condition

\[ \psi_I(b) = 0 \]  

(21)

gives

\[ \theta_b = n\pi \quad \text{for the antisymmetric function} \]  

(22)

\[ \theta_b = \left( n + \frac{1}{2} \right) \pi \quad \text{for the symmetric function} \]  

(23)

where

\[ \theta_b = \int_{0}^{b} \Gamma(x)dx \]  

(24)

\( n = 0, 1, 2, 3, \ldots \)

We apply our formalism to the 1-dimensional (i) harmonic and (ii) quartic oscillators, limited by infinite walls at \( x = \pm b \). Such limited oscillator potentials can be used directly to simulate the lowest excited states of an oscillating system [15].
i) **Harmonic Oscillator (HO)**

The 1-dimensional confined HO is described by the potential

\[
V(x) = \begin{cases} 
  x^2 & \text{for } -b < x < b \\ 
  \infty & \text{for } |x| > b 
\end{cases}
\]

The turning points are at \(x_t = \pm \sqrt{E}\).

We calculate the energy eigenvalues for various values of the confining parameter \(b\), and observe that our results are far better than those obtained by the shifted \(1/N\) expansion method [16] as shown in Table 1. It is also observed (from Table 1) that with the increase of the confinement parameter the vibrational excitation energy of the oscillator decreases, rapidly tending to that of the unlimited oscillator.

ii) **Quartic Oscillator (QO)**

The 1-dimensional confined QO is described by the potential

\[
V(x) = \begin{cases} 
  x^4 & \text{for } -b < x < b \\ 
  \infty & \text{for } |x| > b 
\end{cases}
\]

The turning points are at \(x_t = \pm E^{1/4}\).

The energy eigenvalues are calculated from eqns. (17), (22) and (19), (23) for the antisymmetric and symmetric functions respectively where eqns. (17), (19) are for the turning points lying inside the confining box, and (22), (23) are for the turning points outside the box. The values are given in Table 2, for \(b = 1\), alongside the values obtained by other methods for comparison, explained later on.

iii) **Infinite quantum well subject to an electric field**

This is the interesting problem of an electric field \(F\) being applied on a particle of charge \(-|e|\), bound in an infinite quantum well of width \(b\).

\[
V(x) = \begin{cases} 
  |e|Fx & \text{for } 0 < x < b \\ 
  \infty & \text{for } x > b 
\end{cases}
\]
The boundary conditions are

$$\begin{align*}
\psi(0) &= 0 \\
\psi(b) &= 0
\end{align*}$$

(28)

and the turning point is at

$$x_t = \frac{E}{|e| F}$$

(29)

For $E < |e| F b$, the energy is calculated using eqn. (17), while eqn. (22) determines the energy for $E > |e| F b$.

To simplify calculations, we choose a scaling such that $|e| F = 1$, so that

$$V(x) = x \quad \text{for} \quad 0 < x < b$$

$$\infty \quad \text{for} \quad x > b$$

The results are quoted in Table 3.

### III MAF formalism for confined systems

Though the WKB quantisation rule works well enough for confined systems, the WKB solutions are valid in regions far removed from the turning points. In contrast, the Modified Airy Function (MAF) [23-25] method gives an extremely accurate description of both the eigenfunctions as well as the eigenvalues in the entire region, including the turning point. In this section we shall develop a generalized version of the MAF method, which is suitable for spatially confined quantum mechanical systems. In this connection it may be noted that Spehner et. al. [22] have also considered the Airy function approach to obtain the energies of non-interacting electrons in a magnetic field, constrained to a 2-dim. domain with boundaries. However, in our case, the argument in the Airy function $\xi(x)$ is related to $(E - V(x))^{1/2}$ (see equation (31)) ; only in case of linear $V(x)$, is $\xi(x)$ linearly related to $x$.

We start with the 1-dimensional Schrödinger equation (in units $\hbar = c = 2m = 1$)

$$\frac{d^2 \psi}{dx^2} + \Gamma^2(x) \psi = 0$$

(1)

with

$$\Gamma^2(x) = E - V(x)$$

(2)
The general MAF solution to (1) is of the form
\[ \psi(x) = c_1 \frac{Ai[\xi(x)]}{\sqrt{\xi'(x)}} + c_2 \frac{Bi[\xi(x)]}{\sqrt{\xi'(x)}} \]  
where \( Ai[\xi(x)] \), \( Bi[\xi(x)] \) are the Airy functions defined in [26] and
\[ \xi(x) = -\left\{ \frac{3}{2} \int_x^{x_t} \Gamma(x)dx \right\}^{2/3}; x < x_t \]  
\[ \xi(x) = \left\{ \frac{3}{2} \int_{x_t}^x \kappa(x)dx \right\}^{2/3}; x > x_t \]  
\[ \Gamma^2(x) = -\kappa^2(x) \]  
with \( x_t \) being the turning point (i.e. the point where \( \Gamma^2(x) = 0 \)).

It is to be noted here that the appearance of the term \( Bi[\xi(x)] \) is solely due to confinement. It cannot appear in the unconfined case because of the boundary conditions.

Analogous to the WKB case, we consider only symmetric profiles. Hence the eigenfunctions are either symmetric or antisymmetric in \( x \), obeying boundary conditions
\[ \begin{align*}
\psi'(0) &= 0 \quad \text{for the symmetric function} \\
\psi(0) &= 0 \quad \text{for the antisymmetric function}
\end{align*} \]  
(34)

Also the confining potential is such that it exists only in the region \(-b < x < b\) and is infinite elsewhere. The leads to the boundary condition
\[ \psi(\pm b) = 0 \]  
(35)

Substitution of (34) and (35) in (30) gives the following eigenvalue equation (after some straightforward calculations):

i) for the antisymmetric function
\[ Ai[\xi(0)]. Bi[\xi(b)] - Bi[\xi(0)]. Ai[\xi(b)] = 0 \]  
(36)

ii) for the symmetric function
\[ \{4\xi(0). Ai'[\xi(0)] + Ai[\xi(0)]\}. Bi[\xi(b)] - \{4\xi(0). Bi'[\xi(0)] + Bi[\xi(0)]\}. Ai[\xi(b)] = 0 \]  
(37)
where $A_i'[\xi(x)], B_i'[\xi(x)]$ are the derivatives of $A_i[\xi(x)]$ and $B_i[\xi(x)]$ with respect to $\xi$, respectively. Thus the eigen energies are obtained from (36) and (37) after determining $\xi(0)$ and $\xi(b)$ from (31)-(33) and $A_i(\xi), B_i(\xi), A_i'(\xi), B_i'(\xi)$ etc. from the formulae given in ref.[26]. We have applied our formalism to all the three problems discussed in Section II, and given our results in the various Tables. (The symbols are explained later on.)

IV Results and Discussions

Table 1 gives the first excited state eigenenergies of the 1-dimensional confined HO for different values of the confinement parameter $b$. $E(1/N)$ are the energies obtained by shifted $1/N$ expansion method [16], $E(V)$ are the WKB results of Vawter [21], $E(exV)$ are the exact numerical energies as given in ref.[21], and $E(WKB)$ and $E(MAF)$ are our results by WKB and MAF methods respectively. $E(exact)$ are the exact numerical ground state energies of the 3-dimensional HO confined in a spherical box, from ref. [7]. Strictly speaking, we cannot compare our 1-dimensional results with the 3-dimensional case. However, since the asymptotic ground state energy of the 3-dimensional HO ($l = 0$ case) coincides with the first excited state energy of the 1-dimensional HO, we have assumed the comparison to hold even in cases of confinement. In fact, it is easy to observe from Table 1 that the comparison holds extremely well for $b = 1$ and $b = 2$, i.e. $E(exV) = E(exact)$.

As is observed from Table 1, both WKB and MAF methods give results far superior to the shifted $1/N$ expansion procedure, for various values of the confining parameter $b$. It is interesting to note that our WKB results are better than those of the WKB results of Vawter [21] (for $b = 2$). It is observed that our WKB and MAF results differ very little from each other. As expected, both WKB and MAF energies tend rapidly to those of the unconfined oscillator as the well size gets larger.

Table 2 gives the results of the confined 1-dimensional QO, for $b = 1$ in units of $E_1^\infty = \pi^2/8$. $E(BS)$ and $E(mBS)$ are the energies by Bohr-Sommerfeld quantisation rule, and a matrix formulation of the same respectively [20], $E(Pwr)$ and $E(Var)$ are those
obtained by power series expansion [27] and variational methods [15] respectively. For the numerical results, $E(\text{exact})$, we quote the perturbation results of ref.[28] since it makes no approximation in deriving the equations, and one can compute the eigenvalues to a high degree of accuracy by considering a large number of terms of the infinite series. Our results are denoted by $E(\text{WKB})$ and $E(\text{MAF})$. All the results are quoted after suitable normalization. The variational method [15] gives the best estimates of the energies, followed by power series expansion method [27]. As for comparison among the BS, mBS, WKB and MAF values, the mBS formalism is the best of the lot. The WKB method (correctly applied) gives energies at least as accurate as the BS (Bohr-Sommerfeld) ones, contrary to the claim of Gomes and Adhikari [20]. The MAF method gives marginally better results than either BS or WKB approximations.

Table 3 gives the WKB and MAF energies for a boxed-in charged particle subject to an external electric field $F$. ($V = |e|Fx$ for $x \leq b$, and $\infty$ for $x > b$). Using a suitable scaling, we have taken $|e| F = 1$. $E(\text{exact})$ are the accurate energy eigenvalues from ref.[29]. For this particular case, the MAF method is supposed to give the exact result. However, one has to be very cautious while calculating the values of Airy functions and their derivatives, which are highly oscillatory. An extremely small error may get magnified in the energy eigenvalue. As is observed from Table 3, the WKB quantisation rule gives energies extremely close to the exact values. The MAF values are slightly worse than the WKB ones for extremely small confinement parameter. As the size of the confining box increases, the MAF results get better. It is interesting to mention here that Gomes and Adhikari [20] attempted this problem with a matrix formulation of the Bohr-Sommerfeld (mBS) quantisation rule, claiming WKB does not give good result in this case. Contrary to this claim we observed that the correct WKB method gives quite accurate values, (pretty close to MAF ones). Also the analytical formula given in ref.[20] does not give the correct asymptotic behaviour of energy eigenvalues for large $b$. (Hence we have not given $E(\text{mBS})$ values for $b > 1$.) However, the graph presented in their paper apparently gives values (obtained by mBS method) quite close to the numerical results. As $b$ increases, both WKB and MAF energies tend to the exact energies for the unconfined case, which is nothing but the zeroes of the Airy function.
To conclude, we have developed a formalism for studying spatially confined quantum mechanical systems in the framework of the usual WKB and MAF methods. Confinement imposes certain boundary conditions which modify the asymptotic quantization rules. The methods can be applied to determine the eigenenergies of non-solvable potentials, bound in quantum well structures. To establish the reliability of our formalism we have calculated the eigenenergies of the confined 1-dimensional harmonic and quartic oscillators, and a boxed-in charged particle in an external electric field, and found our results to be pretty close to the accurate numerical values, contrary to the claim regarding WKB method in ref. [20]. In fact, our findings encourage us to hope that WKB and MAF methods would be very useful in studying confined quantum mechanical systems for various boundary conditions.
### Table 1 Harmonic Oscillator \((2m = 1)\)

| \(b\) | \(E(1/N)\) | \(E(WKB)\) | \(E(MAF)\) | \(E(V)\) | \(E(exV)\) | \(E(exact)\) |
|-------|-------------|-------------|-------------|----------|-------------|--------------|
| 0.5   | 40.9612     | 39.5619     | 39.5605     | 39.5490  |              |              |
| 1.0   | 10.5170     | 10.2052     | 10.2050     | 10.20    | 10.15       | 10.1510      |
| 1.5   | 5.2136      | 5.1636      | 5.1635      |          | 5.0100      |              |
| 2.0   | 3.7316      | 3.5374      | 3.5368      | 3.357    | 3.529       | 3.5296       |
| 3.0   | 3.0720      | 3.0129      | 3.0070      |          | 3.0122      |              |
| 5.0   | 3.0000      | 3.0000      | 3.0000      |          | 3.0000      |              |

### Table 2 Quartic Oscillator for \(b = 1\) \((2m = 1)\)

| \(n\) | \(E(mBS)\) | \(E(BS)\) | \(E(Pwr)\) | \(E(Var)\) | \(E(WKB)\) | \(E(MAF)\) | \(E(exact)\) |
|-------|-------------|-------------|-------------|-------------|-------------|-------------|--------------|
| 1     | 2.0901      | 2.1687      | 2.0331      | 2.0314      | 2.1685      | 2.1670      | 2.0317       |
| 2     | 8.0901      | 8.1635      | 8.0920      | 8.0855      | 8.1636      | 8.1198      | 8.0860       |
| 3     | 18.0900     | 18.1628     | 18.0242     | 18.1133     | 18.1628     | 18.1233     | 18.1135      |
| 4     | 32.0900     | 32.1629     | 32.1313     | 32.1165     | 32.1624     | 32.1612     | 32.1165      |

### Table 3 \(V = x\) for \(0 < x \leq b\), and \(\infty\) for \(x > b\) \((2m = 1)\)

| \(b\) | \(E(WKB)\) | \(E(MAF)\) | \(E(mBS)\) | \(E(exact)\) |
|-------|-------------|-------------|-------------|--------------|
| 0.3   | 109.8133    | 109.8223    | 109.6461    | 109.8123     |
| 0.5   | 39.7286     | 39.7314     | 39.4508     | 39.7283      |
| 0.8   | 15.8222     | 15.8232     | 15.3769     | 15.8208      |
| 1.0   | 10.3717     | 10.3716     | 9.8141      | 10.3685      |
| 1.5   | 5.1472      | 5.1471      |              | 5.1309       |
| 2.0   | 3.5017      | 3.5016      |              | 3.4499       |
| 3.0   | 2.5198      | 2.5066      |              | 2.5090       |
| 4.0   | 2.3391      | 2.3404      |              | 2.3555       |
| 5.0   | 2.3382      | 2.3381      |              | 2.3390       |
| 6.0   | 2.3382      | 2.3381      |              | 2.3381       |

### Acknowledgment

The authors are grateful to the referees for some useful comments and suggestions, without which the paper could not have been written in the present form. One of the authors (A.S.) acknowledges financial assistance from the Council of Scientific and Industrial Research, India.
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