

## Langer Modification in WKB Quantization for Translationally Shape Invariant Potentials<sup>†</sup>

Hosung Sun

*Department of Chemistry, Sungkyunkwan University, Suwon 440-746, Korea. E-mail: hsun@skku.edu*  
*Received November 22, 2011, Accepted December 16, 2011*

When the Langer modification is applied to Coulomb potential, the standard WKB quantization yields an exact energy spectrum for the potential. This Langer modification has been known to be related to the centrifugal term appearing in Coulomb potential. But we find that a similar modification exists for all translationally shape invariant potentials without referring to the centrifugal term. The characteristic shape of the potentials accounts for the generalized version of Langer modification that makes the WKB quantization valid for all translationally shape invariant potentials.

**Key Words :** WKB quantization, Langer modification, Shape invariant potentials

### Introduction

It is very important to understand the relation between classical mechanics and quantum mechanics. Numerous researches to search for the relation have been performed and semiclassical theories or approaches are one of such efforts. In the same year when Schrödinger's wave equation of quantum mechanics was published, Wentzel, Kramers, and Brillouin developed a semiclassical approximation now known as the WKB quantization or the WKB approximation.<sup>1-3</sup> The WKB quantization has become a textbook knowledge nowadays.<sup>4,5</sup>

The one-dimensional Schrödinger equation for a bound state under potential  $V(x)$  is, in units of  $2m = \hbar = 1$ ,

$$-\frac{d^2}{dx^2}\Psi_n(x) + V(x)\Psi_n(x) = E_n\Psi_n(x) \quad (1)$$

where  $n$  is the quantum number or a number of nodes in the wave function  $\Psi_n(x)$ . Let  $p_n(x) \equiv \sqrt{E_n - V(x)}$  be the classical momentum function for an energy  $E_n$ , then the well-known standard WKB quantization (or the lowest order WKB approximation) is<sup>4-6</sup>

$$\int_{x_{1,n}}^{x_{2,n}} p_n(x) dx = \int_{x_{1,n}}^{x_{2,n}} \sqrt{E_n - V(x)} dx = (n + 1/2)\pi. \quad (2)$$

$x_{1,n}$  and  $x_{2,n}$  are two classical turning points ( $x_{1,n} < x_{2,n}$ ), i.e.  $V(x_{1,n}) = V(x_{2,n}) = E_n$ .

Since the WKB quantization (2) is the lowest order (i.e. the first order in  $\hbar$  when Hamilton's principal function  $S(x) = -i\hbar \ln \Psi(x)$  is expanded in terms of  $\hbar$ ) approximation, it is not exact in general. But the WKB quantization has been found to be exact for two potentials, i.e. the harmonic oscillator potential and Morse potential. It is because the higher order WKB corrections to the energy quantization condition are shown to be identically zero for the two

potentials. Also using the exact quantization rule which is rather recently found,<sup>7-12</sup> the exactness of WKB quantization for the two potentials has been explained.

For Coulomb potential

$$V(r) = -\frac{e^2}{r} + \frac{l(l+1)}{r^2}, \quad (3)$$

the WKB quantization (2) is, of course, not exact. However, when the quantity  $l(l+1)$  in  $V(r)$  is replaced by  $(l+1/2)^2$ , the WKB quantization provides an exact energy spectrum of the original potential  $V(r)$  in Eq. (3). It was first noted by Uhlenbeck<sup>13</sup> and later reconsidered by Langer.<sup>14</sup> Nowadays this replacement is known as "Langer modification".<sup>15-17</sup> Interestingly the Langer modification is no longer valid when the higher order terms are included into the lowest order WKB quantization (2). The various discussions related to the Langer modification have been reported<sup>18-21</sup> and also applications to actual systems have been carried out.<sup>22-24</sup>

The validity of Langer modification was first explained by Langer for Coulomb potential.<sup>14</sup> He noticed that the radial WKB wave function does not behave properly at the origin  $r=0$ . The Langer modification (i.e.  $l(l+1) \rightarrow (l+1/2)^2$ ) regularizes the WKB wave function at the origin and ensures correct asymptotic behavior at large  $n$  quantum numbers. Another potential for which Langer modification is valid is the 3-D harmonic oscillator potential (also called isotonic oscillator potential),<sup>25</sup> i.e.

$$V(r) = \frac{1}{4}\omega^2 r^2 + \frac{l(l+1)}{r^2}. \quad (4)$$

Notice that Coulomb potential (3) and the 3-D harmonic oscillator potential (4) both are actually the radial part of the three dimensional  $(r, \theta, \phi)$  spherically symmetric potential. The  $l(l+1)/r^2$  term corresponds to the so-called "centrifugal term" which originates from the angular momentum operator  $\hat{L}^2(r, \theta, \phi)$ . Sergeenko derived the lowest order approximation of  $\hat{L}^2(r, \theta, \phi)$  as the lowest order WKB quantization is derived and showed the existence of a new

<sup>†</sup>This paper is to commemorate Professor Kook Joe Shin's honourable retirement.

operator  $\vec{M}^2(r, \theta, \phi)$  in the quasiclassical region.<sup>26</sup> The  $\vec{M}$  has eigenvalues of  $(l+1/2)^2$  while  $\vec{L}^2$  has  $l(l+1)$ . This study more or less justifies the Langer modification.

In short, the WKB quantization is exact for the harmonic oscillator potential and Morse potential. For Coulomb potential and the 3-D harmonic oscillator potential (having the centrifugal term  $l(l+1)/r^2$ ), the WKB quantization becomes exact when Langer modification is introduced. It is summarized in Table 1 with explicit expressions for the four potentials.

When a potential  $V(x; a_2)$  ( $a_2$  is a parameter) and its supersymmetric partner potential  $V^{\text{susy}}(x; a_1)$  (a parameter  $a_1 = a_2 + \text{constant}$ ) have a condition of  $V^{\text{susy}}(x; a_1) = V(x; a_2) + R(a_1)$  (the remainder  $R(a_1)$  is independent of  $x$ ), the two partner potentials are said to be translationally shape invariant. The two partner potentials have a common shape. A potential that satisfies the above condition is called "translationally shape invariant potential (TSIP)".<sup>27</sup> We notice that all of the four potentials under discussion are TSIP. We have examined other TSIP to see if there is a similarly valid modification to the WKB quantization and found that there, indeed, is a Langer-like modification for all TSIP. This is because all other TSIP, though they do not explicitly have a centrifugal term, have a formally similar term like the centrifugal term of Coulomb potential.

In the next section the reason why the Langer modification is valid for Coulomb and the 3-D harmonic oscillator potentials is explained by using the exact quantization rule. This section also suggests an interesting clue for finding a similar modification for other TSIP. In the following two sections the modifications for other TSIP are derived and the relationship between the shape of TSIP and the modification is discussed. Conclusion and discussions are provided in the last section.

**Table 1.** Langer modification (LM).  $\gamma$  is the correction term (Eqs. 9 and 10). The eigenvalues ( $E_n$ ) are given in units of  $2m = \hbar = 1$ . The constants  $A, B, b, \alpha, \omega, l$  are all taken  $\geq 0$ . The range of potentials is  $-\infty \leq x \leq \infty, 0 \leq r \leq \infty$ .

Harmonic oscillator	
$V(x) = \frac{1}{4}\omega^2\left(x - \frac{2b}{\omega}\right)^2$	$E_n = (n+1/2)\omega$
$\gamma = 0$	LM: not required
Morse	
$V(x) = B^2 \exp(-2\alpha x) - 2B(A + \alpha/2) \exp(-\alpha x)$	$E_n = -(A - n\alpha)^2$
$\gamma = 0$	LM: not required
Coulomb	
$V(r) = -\frac{e^2}{r} + \frac{l(l+1)}{r^2}$	$E_n = -\frac{e^4}{4(n+l+1)^2}$
$\gamma = \pi\left(l + \frac{1}{2} - \sqrt{l(l+1)}\right)$	LM: $l(l+1) \rightarrow (l+1/2)^2$
3-D harmonic oscillator	
$V(r) = \frac{1}{4}\omega^2 r^2 + \frac{l(l+1)}{r^2}$	$E_n = (2n+l+3/2)\omega$
$\gamma = \frac{\pi}{2}\left(l + \frac{1}{2} - \sqrt{l(l+1)}\right)$	LM: $l(l+1) \rightarrow (l+1/2)^2$

## Langer Modification for Coulomb Potential

The Langer modification is

$$l(l+1) \rightarrow (l+1/2)^2. \quad (5)$$

The Langer modified Coulomb potential  $V^{\text{Mod}}(r)$  can be obtained by inserting the modification (5) into the original Coulomb potential (3), i.e.

$$V^{\text{Mod}}(r) = -\frac{e^2}{r} + \frac{(l+1/2)^2}{r^2}. \quad (6)$$

The modified WKB integral (i.e. half-action integral in phase space) in Eq. (2) can be easily evaluated as

$$\begin{aligned} \int_{r_{1,n}}^{r_{2,n}} \sqrt{E_n - V^{\text{Mod}}(r)} dr &= \int_{r_{1,n}}^{r_{2,n}} \sqrt{E_n - \left[-\frac{e^2}{r} + \frac{(l+1/2)^2}{r^2}\right]} dr \\ &= \pi(e^2/\sqrt{-4E_n} - l - 1/2) \end{aligned} \quad (7)$$

Using the WKB quantization (2), i.e. Eq. (7)  $= (n+1/2)\pi$ , one can evaluate the energy  $E_n$ ,

$$E_n = -\frac{e^4}{4(n+l+1)^2}. \quad (8)$$

Indeed Eq. (8) is the exact energy expression for the original Coulomb potential  $V(r)$  in Eq. (3). It shows that the exact energy for Coulomb potential can be obtained from the WKB quantization with Langer modification.

As mentioned in the previous section, the exact quantization rule for one-dimensional quantum systems has been found. There is a class of potentials called translationally shape invariant potentials which are exactly solvable. For TSIP the exact quantization rule can be written as<sup>7-12,28,29</sup>

$$\int_{x_{1,n}}^{x_{2,n}} \sqrt{E_n - V(x)} dx = (n+1/2)\pi + \gamma \quad (9)$$

with

$$\gamma = \frac{1}{2}\pi + \int_{x_{1,0}}^{x_{2,0}} \frac{W(x)}{dW(x)/dx} \left( \frac{dp_0(x)}{dx} \right) dx. \quad (10)$$

The superpotential is the minus logarithmic derivative of the ground state ( $n=0$ ) wave function  $\Psi_0(x)$ , i.e.

$$W(x) = -\frac{d\Psi_0(x)/dx}{\Psi_0(x)} \quad (11)$$

and the ground state momentum function  $p_0(x) = \sqrt{E_0 - V(x)}$ .  $x_{1,0}$  and  $x_{2,0}$  are two classical turning points ( $x_{1,0} < x_{2,0}$ ) for the ground state, i.e.  $V(x_{1,0}) = V(x_{2,0}) = E_0$ . The correction term  $\gamma$  is, in general, energy (or  $n$ ) dependent but it is a constant for TSIP.

Note that the exact quantization rule (9) is reduced to the WKB quantization (2) when the correction term  $\gamma$  is zero, which means the WKB quantization is exact when  $\gamma = 0$ . For the harmonic oscillator and Morse potentials,  $\gamma$  turns out to be zero so that the WKB quantization is exact for the two potentials.<sup>7</sup>

Let us examine the Coulomb potential case by evaluating the correction term  $\gamma$ . Since the ground state energy is (see Table 1)  $E_0 = -\frac{e^4}{4(l+1)^2}$ ,  $p_0(r)$  is

$$p_0(r) = \sqrt{-\frac{e^4}{4(l+1)^2} - \left[-\frac{e^4}{r} + \frac{l(l+1)}{r^2}\right]} = \sqrt{\frac{e^4 l^2}{4C^2} + \frac{e^2}{r} - \frac{C}{r^2}} \quad (12)$$

with  $C \equiv l(l+1)$ .

The superpotential for Coulomb potential is known as<sup>27</sup>

$$W(r) = \frac{e^2}{2(l+1)} - \frac{l+1}{r} = \frac{e^2 l}{2C} - \frac{C}{lr}. \quad (13)$$

Therefore the correction term  $\gamma$ , from Eq. (10), is

$$\begin{aligned} \gamma &= \frac{1}{2}\pi + \int_{r_{1,0}}^{r_{2,0}} \left( \frac{e^2 l}{2C} - \frac{C}{lr} \right) \left[ \frac{d}{dr} \left( \frac{e^2 l}{2C} - \frac{C}{lr} \right) \right]^{-1} \left[ \frac{d}{dr} \sqrt{\frac{e^4 l^2}{4C^2} + \frac{e^2}{r} - \frac{C}{r^2}} \right] dr \\ &= \pi \left( \frac{1}{2} + l - \sqrt{C} \right) \end{aligned} \quad (14)$$

(In the present article, to avoid complexity, we do not present the integration procedure in details. All of the integrations under discussion are straight forward though time consuming.) Since  $C = l(l+1)$  for Coulomb potential, one obtains

$$\gamma = \pi \left( l + \frac{1}{2} - \sqrt{l(l+1)} \right) \quad (15)$$

as listed in Table 1. Clearly  $\gamma$  is not zero so that the WKB quantization is *not valid* for Coulomb potential.

Now let us introduce the Langer modification, i.e.  $C = (l + 1/2)^2$ . Inserting it into Eqs. (12) and (13), one finds that  $\gamma$  is zero (see Eq. (14)). It explains, if not proves, why the WKB quantization with the Langer modification of  $l(l+1) \rightarrow (l + 1/2)^2$  is *valid* for Coulomb potential. The same argument holds for the 3-D harmonic oscillator potential, too.

At this point one may make an interesting observation. If one wants to find a modification, the modification can be easily guessed by examining solely  $\gamma$  of the original potential, i.e. reevaluation of  $\gamma$  for the modified potential is not necessary. In the current example of Coulomb potential, evaluation of Eq. (14) with  $C = (l + 1/2)^2$  is not necessary. Instead, the original  $\gamma$  (Eq. 15) is sufficient enough to find an appropriate modification. To emphasize this observation, let us examine the 3-D harmonic oscillator potential. For this potential, the correction term is  $\gamma = (\pi/2)(l + 1/2 - \sqrt{l(l+1)})$ . By simply looking at the form of  $\gamma$ , one can easily find the modification of  $l(l+1) \rightarrow (l + 1/2)^2$ , which yields  $\gamma = 0$ . Indeed it is the Langer modification for the 3-D harmonic oscillator potential. Using this observation as a clue, we will find an appropriate modification for other TSIP in the following section.

### Langer Modification for TSIP

The Langer modification has been considered and found to be valid only for Coulomb and the 3-D harmonic oscillator potentials that have the centrifugal term  $l(l+1)/r^2$ . Now we would like to search other TSIP for which the Langer modification (or a similar modification) may be valid. From the observation discussed in the previous section, one learns that a modification (if there is any) can be found by simply

examining the correction term of a potential.

For example, generalized Pöschl-Teller potential is

$$\begin{aligned} V(r) &= (A^2 + B^2 + A\alpha) \operatorname{cosech}^2 \alpha r - B(2A + \alpha) \coth \alpha r \operatorname{cosech} \alpha r \\ &= \frac{1}{2} [(B+A)(B+A+\alpha) + (B-A)(B-A-\alpha)] \operatorname{cosech}^2 \alpha r \\ &\quad - B(2A + \alpha) \coth \alpha r \operatorname{cosech} \alpha r \end{aligned} \quad (16)$$

where  $A$ ,  $B$ , and  $\alpha$  are potential parameters. The superpotential and the ground state energy are  $W(r) = A \coth \alpha r - B \operatorname{cosech} \alpha r$  and  $E_0 = -A^2$ . Then the correction term  $\gamma$  (Eq. 10) is

$$\gamma = \frac{\pi}{\alpha} \left[ -A - \frac{1}{2}\alpha + \frac{1}{2}\sqrt{(B+A)(B+A+\alpha)} - \frac{1}{2}\sqrt{(B-A)(B-A-\alpha)} \right] \quad (17)$$

Examining Eq. (17), one easily finds that when  $(B+A)(B+A+\alpha)$  is replaced by  $(B+A+\alpha/2)^2$  and  $(B-A)(B-A-\alpha)$  is replaced by  $(B-A-\alpha/2)^2$  the correction term  $\gamma$  is zero, i.e.

$$\gamma = \frac{\pi}{\alpha} \left[ -A - \frac{1}{2}\alpha + \frac{1}{2}\sqrt{(B+A+\alpha/2)^2} - \frac{1}{2}\sqrt{(B-A-\alpha/2)^2} \right] = 0. \quad (18)$$

The WKB integral with the replacement is

$$\begin{aligned} &\int_{r_{1,n}}^{r_{2,n}} \sqrt{E_n - V^{\text{Mod}}(r)} dr \\ &= \int_{r_{1,n}}^{r_{2,n}} \sqrt{E_n - \left[ \frac{1}{2} \{ (B+A+\alpha/2)^2 + (B-A-\alpha/2)^2 \} \operatorname{cosech}^2 \alpha r \right.} \\ &\quad \left. - B(2A + \alpha) \coth \alpha r \operatorname{cosech} \alpha r \right]} dr \quad (19) \\ &= \frac{\pi}{\alpha} (A + \alpha/2 - \sqrt{-E_n}). \end{aligned}$$

Then the WKB quantization of

$$\frac{\pi}{\alpha} (A + \alpha/2 - \sqrt{-E_n}) = (n + 1/2)\pi \quad (20)$$

yields the energy  $E_n = -(A - n\alpha)^2$  that is the *exact* energy expression for generalized Pöschl-Teller potential. It verifies that the replacement of  $(B+A)(B+A+\alpha) \rightarrow (B+A+\alpha/2)^2$  and  $(B-A)(B-A-\alpha) \rightarrow (B-A-\alpha/2)^2$  is an appropriate Langer-like modification which we call “generalized Langer modification”.

We present Scarf II potential, as another example, because the correction term (or a quantity similar to it) has never been reported before. Scarf II potential is

$$\begin{aligned} V(x) &= [B^2 - A(A+\alpha) \operatorname{sech}^2 \alpha x + B(2A + \alpha) \operatorname{sech} \alpha x \tanh \alpha x], \quad (21) \\ W(x) &= A \tanh \alpha x + B \operatorname{sech} \alpha x, \end{aligned}$$

and  $E_0 = -A^2$ .

The correction term  $\gamma$  is, i.e.

$$\begin{aligned} \gamma &= \frac{1}{2}\pi + \int_{x_{1,0}}^{x_{2,0}} \frac{A \tanh \alpha x + B \operatorname{sech} \alpha x}{\frac{d}{dx} (A \tanh \alpha x + B \operatorname{sech} \alpha x)} \\ &\quad \otimes \frac{d}{dx} \sqrt{-A^2 - [B^2 - A(A+\alpha)] \operatorname{sech}^2 \alpha x - B(2A + \alpha) \operatorname{sech} \alpha x \tanh \alpha x} dx \\ &= \frac{\pi}{\alpha} \left[ -A - \frac{1}{2}\alpha + \frac{1}{\sqrt{2}} \left[ \sqrt{[A(A+\alpha)]^2 + B^4 - 2B^2 A(A+\alpha) + 4B^2 (A+\alpha/2)^2} \right]^{1/2} \right. \\ &\quad \left. + A(A+\alpha) - B^2 \right] \\ &= \frac{\pi}{2\alpha} [-2A - \alpha - \sqrt{(-A+iB)(-A-iB-\alpha)} - \sqrt{(-A-iB)(-A-iB-\alpha)}]. \quad (22) \end{aligned}$$

When the replacement of

$$(-A+iB)(-A+iB-\alpha) \rightarrow (-A+iB-\alpha/2)^2$$

and

$$(-A-iB)(-A-iB-\alpha) \rightarrow (-A-iB-\alpha/2)^2 \quad (23)$$

is made, the correction term becomes zero, i.e.

$$\gamma = \frac{\pi}{2\alpha} \left[ -2A - \alpha - \sqrt{(-A+iB-\alpha/2)^2} - \sqrt{(-A-iB-\alpha/2)^2} \right] = 0 \quad (24)$$

The WKB integral is evaluated to verify if this replacement (Eq. 23) makes the WKB quantization exact. One finds that

$$A(A+\alpha) = B^2 + [(-A+iB)(-A+iB-\alpha) + (-A-iB)(-A-iB-\alpha)]/2. \quad (25)$$

When the replacement (Eq. 23) is made, the R.H.S. of Eq. (25) becomes

$$B^2 + [(-A+iB)(-A+iB-\alpha) + (-A-iB)(-A-iB-\alpha)]/2 \rightarrow B^2 + [(-A+iB-\alpha/2)^2 + (-A-iB-\alpha/2)^2]/2 = (A+\alpha/2)^2. \quad (26)$$

It means that the replacement (Eq. 23) is equivalent to the replacement of

$$A(A+\alpha) \rightarrow (A+\alpha/2)^2. \quad (27)$$

Instead of using the original replacement (Eq. 23), one can use the equivalent replacement (Eq. 27), i.e.

$$\begin{aligned} & \int_{x_{1,n}}^{x_{2,n}} \sqrt{E_n - V^{\text{Mod}}(x)} \, (dx) \\ &= \int_{x_{1,n}}^{x_{2,n}} \sqrt{E_n - \{B^2 - (A + \alpha/2)^2\} \operatorname{sech}^2 \alpha x + B(2A + \alpha) \operatorname{sech} \alpha x \tanh \alpha x} \, dx \\ &= \frac{\pi}{\alpha} (A + \alpha/2 - \sqrt{-E_n}). \end{aligned} \quad (28)$$

The WKB quantization of

$$\frac{\pi}{\alpha} (A + \alpha/2 - \sqrt{-E_n}) = (n + 1/2)\pi \quad (29)$$

yields the energy  $E_n = -(A - n\alpha)^2$ , that is *exact* energy expression for Scarf II potential. It verifies that  $(-A+iB)(-A+iB-\alpha) \rightarrow (-A+iB-\alpha/2)^2$  and  $(-A-iB)(-A-iB-\alpha) \rightarrow (-A-iB-\alpha/2)^2$  is a generalized Langer modification or simply it is  $A(A+\alpha) \rightarrow (A+\alpha/2)^2$ .

The “generalized Langer modification” can be summarized as follows. When there is a one-dimensional potential that has  $P_1(P_1+P_2)$  term in a potential function, the modification is

$$P_1(P_1+P_2) \rightarrow (P_1+P_2/2)^2 \quad (30)$$

where  $P_1$  (or  $P_2$ ) is a constant or a parameter (or a combination of parameters) appearing in a potential. For Coulomb potential, one finds that  $P_1 = l$  and  $P_2 = 1$ . One clearly sees that the Langer modification is a special case of the generalized Langer modification. There are two modifications for generalized Pöschl-Teller potential, i.e. ( $P_1 = B+A$ ,  $P_2 = \alpha$ ) and ( $P_1 = B-A$ ,  $P_2 = -\alpha$ ). For Scarf II potential,  $P_1 = A$  and  $P_2 = \alpha$ . We have performed similar analyses on all known translationally shape invariant

potentials<sup>27,28</sup> and the results are summarized in Table 2.

### Generalized Langer Modification and Shape of Potentials

For all TSIP examined in the present work the “Langer modification” or “generalized Langer modification” is found to be valid. Why is it so? An immediate answer may be that Langer modification is valid because all TSIP are exactly solvable. There are other exactly solvable potentials called Natanzon potentials which are not shape invariant.<sup>30-32</sup> The simple WKB quantization (2) cannot be used for Natanzon potentials because they in general have more than two classical turning points. Without the WKB quantization naturally Langer modification is meaningless. Consequently, the solvability of TSIP has nothing to do with the validity of Langer modification.

The potentials in Tables 1 and 2 are all TSIP, i.e. they are shape invariant. “Shape invariant” means that a potential function and its supersymmetric partner potential function have the same form. For details about TSIP, please consult Ref. 27. Then, the shape of potential must be strongly related to the Langer modification. It has been known that all TSIP can be classified into some categories by their shape.<sup>33,34</sup> According to Grandati and Bérard, there should exist a change of variable  $x \rightarrow y$  transforming the original TSIP potential  $V(x)$  into  $V(y)$ .<sup>10,35</sup> Then the whole set of TSIP can be shared in two categories, i.e. a harmonic one and an isotonic one.

The harmonic one (Class I) has a general form of

$$V(y) = \lambda_2 y^2 + \lambda_1 y + \lambda_0. \quad (31)$$

Then the two partner potentials have a form of

$$V_{\pm}(y; a) = a(a - \beta)(y - y_0)^2 + V_0(a) \quad (\text{Class I-1})$$

with the Riccati equation of  $\frac{dy}{dx} = \beta + \beta y^2(x)$  and

$$V_{\pm}(y; a) = a(a + \beta)(y - y_0)^2 + V_0(a) \quad (\text{Class I-2})$$

with  $\frac{dy}{dx} = \beta - \beta y^2(x)$

where  $y_0$  and  $V_0(a)$  are proper constants.

The isotonic one (Class II) has a form of

$$V(y) = \lambda_2 y^2 + \lambda_0 + \mu_2/y^2 \quad (32)$$

and the two partner potentials have a form of

$$V_{\pm}(y; a, b) = a(a - \beta)y^2 + \frac{b(b - \beta)}{y^2} + V_{0\pm}(a, b) \quad (\text{Class II-1})$$

with  $\frac{dy}{dx} = \beta + \beta y^2(x)$  and

$$V_{\pm}(y; a, b) = a(a + \beta)y^2 + \frac{b(b - \beta)}{y^2} + V_{0\pm}(a, b) \quad (\text{Class II-1})$$

with  $\frac{dy}{dx} = \beta - \beta y^2(x)$

**Table 2.** Generalized Langer modification (GLM) for TSIP.  $\gamma$  is the correction term (Eqs. 9 and 10). The eigenvalues ( $E_n$ ) are given in units of  $2m=\hbar=1$ . The constants  $A, B, \alpha$  are all taken  $\geq 0$ . Unless otherwise stated, the range of potentials is  $-\infty \leq x \leq \infty, 0 \leq r \leq \infty$ . For the details of each potential, see Ref. 27.

Rosen-Morse I (trigonometric)

$$V(x) = A(A-\alpha)\operatorname{cosec}^2 \alpha x + 2B\cot \alpha x \quad (0 \leq \alpha x \leq \pi)$$

$$E_n = (A+n\alpha)^2 - B^2/(A+n\alpha)^2$$

$$\gamma = \frac{\pi}{\alpha} \left[ A - \frac{\alpha}{2} - \sqrt{A(A-\alpha)} \right]$$

$$\text{GLM: } A(A-\alpha) \rightarrow (A-\alpha/2)^2$$

Eckart

$$V(x) = A(A-\alpha)\operatorname{cosech}^2 \alpha x - 2B\coth \alpha x \quad (B > A^2)$$

$$E_n = -(A+n\alpha)^2 - B^2/(A+n\alpha)^2$$

$$\gamma = \frac{\pi}{\alpha} \left[ A - \frac{\alpha}{2} - \sqrt{A(A-\alpha)} \right]$$

$$\text{GLM: } A(A-\alpha) \rightarrow (A-\alpha/2)^2$$

Rosen-Morse II (hyperbolic)

$$V(x) = A(A+\alpha)\operatorname{sech}^2 \alpha x + 2B\tanh \alpha x \quad (B < A^2)$$

$$E_n = -(A-n\alpha)^2 - B^2/(A-n\alpha)^2$$

$$\gamma = \frac{\pi}{\alpha} \left[ -A - \frac{\alpha}{2} + \sqrt{A(A+\alpha)} \right]$$

$$\text{GLM: } A(A+\alpha) \rightarrow (A+\alpha/2)^2$$

Scarf I (trigonometric)

$$V(x) = (A^2+B^2-A\alpha)\sec^2 \alpha x - B(2A-\alpha) \tan \alpha x \sec \alpha x$$

$$\left( -\frac{1}{2}\pi \leq \alpha x \leq \frac{1}{2}\pi, A > B \right)$$

$$E_n = (A+n\alpha)^2$$

$$\gamma = \frac{\pi}{2\alpha} [2A - \alpha - \sqrt{(A+B)(A+B-\alpha)} - \sqrt{(A-B)(A-B-\alpha)}]$$

$$\text{GLM: } (A+B)(A+B-\alpha) \rightarrow (A+B-\alpha/2)^2 \text{ \& } (A-B)(A-B-\alpha) \rightarrow (A-B-\alpha/2)^2$$

Scarf II (hyperbolic)

$$V(x) = [B^2 - A(A+\alpha)]\operatorname{sech}^2 \alpha x + B(2A+\alpha) \operatorname{sech} \alpha x \tanh \alpha x$$

$$E_n = -(A-n\alpha)^2$$

$$\gamma = \frac{\pi}{2\alpha} \left[ -2A - \alpha + \sqrt{2} \left[ \sqrt{\frac{[A(A+\alpha)]^2 + B^4 - 2B^2 A(A+\alpha)}{+4B^2(A+\alpha/2)^2}} + A(A+\alpha) - B^2 \right]^{1/2} \right]$$

$$= \frac{\pi}{2\alpha} [-2A - \alpha - \sqrt{(-A+iB)(-A+iB-\alpha)} - \sqrt{(-A-iB)(-A-iB-\alpha)}]$$

$$\text{GLM: } A(A+\alpha) \rightarrow (A+\alpha/2)^2 \text{ or}$$

$$(-A+iB)(-A+iB-\alpha) \rightarrow (-A+iB-\alpha/2)^2 \text{ \& } (-A-iB)(-A-iB-\alpha) \rightarrow (-A-iB-\alpha/2)^2$$

Generalized Pöschl-Teller

$$V(r) = 1/2[(B+A)(B+A+\alpha) + (B-A)(B-A-\alpha)\operatorname{cosech}^2 \alpha r - B(2A+\alpha) \coth \alpha r \operatorname{cosech} \alpha r \quad (A < B)$$

$$E_n = -(A-n\alpha)^2$$

$$\gamma = \frac{\pi}{2\alpha} [-2 - \alpha + \sqrt{(B+A)(B+A+\alpha)} - \sqrt{(B-A)(B-A-\alpha)}]$$

$$\text{GLM: } (B+A)(B+A-\alpha) \rightarrow (B+A-\alpha/2)^2 \text{ \& } (B-A)(B-A-\alpha) \rightarrow (B-A-\alpha/2)^2$$

where  $V_{0+}(a)$  and  $V_{0-}(a)$  are proper constants. The “Class” is categorized by a “shape of potential”.

Grandati and Bérard evaluated the half-action variable for a classical periodic orbit of energy  $E_n$  (which is called the WKB integral in the present work) for various forms of TSIP by using complex analysis.<sup>10,35</sup> Following their complex analysis methodology closely we evaluated the correction term  $\gamma$  and found an appropriate replacement that gives  $\gamma=0$ .

For Class I-1,

$$\gamma = \frac{\pi}{\beta} \left[ a - \frac{1}{2}\beta - \sqrt{a(a-\beta)} \right] \quad (33)$$

and  $\gamma=0$  when  $a(a-\beta) \rightarrow (a-\beta/2)^2$ ,  
for Class I-2,

$$\gamma = \frac{\pi}{\beta} \left[ -a - \frac{1}{2}\beta + \sqrt{a(a+\beta)} \right] \quad (34)$$

and  $\gamma=0$  when  $a(a+\beta) \rightarrow (a+\beta/2)^2$ ,  
for Class II-1,

$$\gamma = \frac{\pi}{2\beta} \left( a - \frac{\beta}{2} - \sqrt{a(a-\beta)} \right) + \frac{\pi}{2\beta} \left( b - \frac{\beta}{2} - \sqrt{b(b-\beta)} \right) \quad (35)$$

and  $\gamma=0$  when  $a(a-\beta) \rightarrow (a-\beta/2)^2$  and  $b(b-\beta) \rightarrow (b-\beta/2)^2$ ,  
and for Class II-2,

$$\gamma = -\frac{\pi}{2\beta} \left( a + \frac{\beta}{2} - \sqrt{a(a+\beta)} \right) + \frac{\pi}{2\beta} \left( b - \frac{\beta}{2} - \sqrt{b(b-\beta)} \right) \quad (36)$$

and  $\gamma=0$  when  $a(a+\beta) \rightarrow (a+\beta/2)^2$  and  $b(b-\beta) \rightarrow (b-\beta/2)^2$ .

As an example, Rosen-Morse I potential is examined, i.e.

$$V(x) = A(A-\alpha)\operatorname{cosec}^2 \alpha x + 2B \cot \alpha x. \quad (37)$$

Let  $y = -\cot \alpha x$ , then one obtains  $V(y) = A(A-\alpha)y^2 - 2By + A(A-\alpha)$  and  $dy/dx = \alpha + \alpha y^2$ . One immediately notices that it belongs to Class I-1 with  $a = A$  and  $\beta = \alpha$ . Then, from Eq. (33), the correction term is  $\gamma = (\pi/\alpha)[A - A/2 - \sqrt{A(A-\alpha)}]$  that is identical with the one (which was obtained by examining the form of  $\gamma$ ) in Table 2. The generalized Langer modification, from Eq. (33), is  $A(A-\alpha) \rightarrow (A-\alpha/2)^2$ .

Following the similar procedure above, we find that Eckart potential belongs to Class I-1 with  $a = A$  and  $\beta = \alpha$ . Rosen-Morse II potential belongs to Class I-2 with  $a = A$  and  $\beta = \alpha$ . Scarf I potential belongs to Class II-1 with  $a = A+B$ ,  $b = A-B$  and  $\beta = \alpha$ . Scarf II potential belongs to Class II-1 with  $a = -A+iB$ ,  $b = -A-iB$  and  $\beta = \alpha$ . Generalized Pöschl-Teller potential belongs to Class II-2 with  $a = B+A$ ,  $b = B-A$ , and  $\beta = \alpha$ .

We have shown that all the shape invariant potentials in Table 2 have a similar formal structure and a similar modification. Therefore, in conclusion, the “shape of potential” is a critical factor to decide whether there exists “generalized Langer modification” or not.

Using the current complex analysis method, now let us examine Coulomb and the 3-D harmonic oscillator potentials for which the Langer modification is valid. For Coulomb potential of  $V(r) = -e^2/r + l(l+1)/r^2$ , the change of variable is  $y = 1/r$  so that  $V(y) = l(l+1)y - e^2y$  and  $dy/dr = -y^2$ . This

potential belongs to Class I but neither to Class I-1 nor to Class I-2. Direct complex analysis (whose methodology is the same as that for Class I-1) results in the correction term  $\gamma = \pi(l+1/2 - \sqrt{l(l+1)})$ . For the 3-D harmonic oscillator potential of  $V(x) = (\omega^2/4)r^2 + l(l+1)/r^2$ , the change of variable is not necessary, i.e.  $y = r$ .  $V(y) = (\omega^2/4)r^2 + l(l+1)/r^2$  and  $dy/dr = 1$ . This potential belongs to Class II but neither to Class II-1 nor to Class II-2. A similar direct complex analysis (whose methodology is the same as that for Class II-1) results in the correction term  $\gamma = \frac{\pi}{2}(l+1/2 - \sqrt{l(l+1)})$ . Therefore, for Coulomb and the harmonic oscillator potentials, the well-known “Langer modification” of  $l(l+1) \rightarrow (l+1/2)^2$  makes the WKB quantization exact.

Finally let us examine the harmonic oscillator and Morse potentials for which Langer modification is not required, i.e. the WKB quantization is exact for these potentials. Since the harmonic oscillator potential is  $V(x) = (\omega^2/4)(x-2b/\omega^2)$ , the change of variable is not necessary, i.e.  $y = x$ .  $V(x) = (\omega^2/4)(x-2b/\omega^2)^2 = (\omega^2/4)y^2 - b\omega y + b^2$  and  $dy/dx = 1$ . For Morse potential, the change of variable is  $y = \exp(-\alpha x)$  so that  $V(y) = B^2 y^2 - 2B(A+\alpha/2)y$  and  $dy/dx = -\alpha y$ . These potentials belong to Class I but neither to Class I-1 nor to Class I-2. Direct complex analysis results in the correction term  $\gamma = 0$ . So that the Langer modification is not required, i.e. the WKB quantization itself provides an exact energy spectrum.

### Conclusion and Discussions

Though the WKB quantization is approximate, it is often, due to its simplicity, used to calculate the energy spectrum of quantum systems. For Coulomb potential system, when Langer modification is introduced, the WKB quantization becomes exact and consequently exact energy can be obtained. So far Coulomb and the 3-D harmonic oscillator potentials are only ones for which the Langer modification of  $l(l+1) \rightarrow (l+1/2)^2$  is valid. We have found a more general form of modification of  $P_1(P_1+P_2) \rightarrow (P_1+P_2/2)^2$  (named “generalized Langer modification”) for all translationally shape invariant potentials including Coulomb potential. Naturally it is sure that the current finding broadens the applicability of the WKB quantization.

When a potential, e.g. Coulomb potential, has a centrifugal term  $l(l+1)/r^2$ , certainly the Langer modification can be explained by the notion that an approximate form of angular momentum operator  $\vec{L}^2$  whose eigenvalue is  $l(l+1)$  is embedded within the WKB quantization. But the current finding dictates that the generalized Langer modification is still valid for other translationally shape invariant potentials that do not have a centrifugal term. We have explained (if not proved) why the generalized Langer modification should be valid for all translationally shape invariant potentials. The reason is that the Langer modification is related to the “shape” of potentials, i.e. all translationally shape invariant potentials have a similar form which is suitable for Langer modification.

Though we have not provided a concrete proof for more fundamental question – “why do translationally shape

invariant potentials have a shape for which the Langer modification can be defined?”, the current finding can be utilized for answering other interesting questions in this field. For example, the well-known supersymmetric WKB quantization,<sup>27</sup> i.e.

$$\int_{x_{1,n}}^{x_{2,n}} \sqrt{E_n - W^2(x)} dx = n\pi, \quad (38)$$

is found to be exact for all translationally shape invariant potentials. This mystery has never been algebraically proved even though there were many attempts. Comparing Eq. (38) with the exact quantization rule (9), one immediately notices that if the correction term  $\gamma$  is  $-\pi/2$  when the potential  $V(x)$  is replaced by  $W^2(x)$ , the supersymmetric WKB quantization must be exact.

For example, Rosen-Morse I potential (Eq. 37) has the correction term  $\gamma$  (see Table 2), i.e.

$$\gamma = \frac{\pi}{\alpha} \left[ A - \frac{\alpha}{2} - \sqrt{A(A-\alpha)} \right]. \quad (39)$$

Note that  $\gamma$  is equal to  $-\pi/2$  when  $A(A-\alpha)$  is replaced with  $A^2$  in Eq. (39). Therefore, one finds that the following quantization should be *exact*, i.e.

$$\int_{x_{1,n}}^{x_{2,n}} \sqrt{E_n - V^{\text{Mod}}(x)} dx = n\pi \quad (40)$$

where

$V^{\text{Mod}}(x) = A^2 \operatorname{cosec}^2 \alpha x + 2B \cot \alpha x$  which is obtained from replacement of  $A(A-\alpha) \rightarrow A^2$  into the original  $V(x)$  of Eq. (37). Since the superpotential for Rosen-Morse I potential is  $W(x) = -A \cot \alpha x - B/A$ , then

$$\begin{aligned} E_n - W^2(x) &= E_0 - (-A \cot \alpha x - B/A)^2 \\ &= A^2 \operatorname{cosec}^2 \alpha x + 2B \cot \alpha x = E_n - V^{\text{Mod}}(x). \end{aligned} \quad (41)$$

Consequently the exact quantization (40) is identical with the supersymmetric WKB quantization (38). It shows that the supersymmetric WKB quantization with modification of  $A(A-\alpha) \rightarrow A^2$  becomes exact for Rosen-Morse I potential. This example suggests that the supersymmetric WKB quantization can be derived from the exact WKB quantization with a proper Langer modification. Full report on this subject will appear elsewhere in the near future.

**Acknowledgments.** This article is dedicated to Professor Kook Joe Shin who is retiring from the lifelong research and education in chemistry. I remember him as an excellent and very fruitful physical chemist as well as a respected human being. It is greatly appreciated that Prof. Shin has showed an immense interest in our group’s research works and encouraged us all the way.

### References

1. Wentzel, G. Z. *Physik* **1926**, 38, 518.
2. Kramers, H. A. Z. *Physik* **1926**, 39, 828.
3. Brillouin, L. C. R. *Hebd. Acad. Sci.* **1926**, 183, 24.
4. Fröman, N.; Fröman, P. O. *JWKB Approximation*; North Holland: Amsterdam, 1965.

5. Merzbacher, E. *Quantum Mechanics*; Wiley: New York, 1970.
  6. Friedrich, H.; Trost, J. *Phys. Rep.* **2004**, 397, 359.
  7. Ou, F. C.; Cao, Z. Q.; Shen, Q. S. *J. Chem. Phys.* **2004**, 121, 8175.
  8. Ma, Z. Q.; Xu, B. W. *Int. J. Modern Phys. E* **2005**, 14, 599.
  9. Ma, Z. Q.; Xu, B. W. *Europhys. Lett.* **2005**, 69, 685.
  10. Grandati, Y.; Bérard, A. *Phys. Lett. A* **2011**, 375, 390.
  11. Qiang, W. C.; Dong, S. H. *Europhys. Lett.* **2010**, 89, 10003.
  12. Dong, S. H.; Morales, D.; García-Ravelo, J. *Int. J. Modern Phys. E* **2007**, 16, 189.
  13. Young, L. A.; Uhlenbeck, G. E. *Phys. Rev.* **1930**, 36, 1158.
  14. Langer, R. E. *Phys. Rev.* **1937**, 51, 669.
  15. Berry, M. V.; Mount, K. E. *Rep. Prog. Phys.* **1972**, 35, 315.
  16. Landau, L. D.; Lifshitz, E. M. *Quantum Mechanics*; Pergamon: Oxford, 1965.
  17. Friedrich, H.; Trost, J. *Phys. Rev. Lett.* **1996**, 26, 4869.
  18. Hur, J.; Lee, C. *Ann. Phys.* **2003**, 305, 28.
  19. Moritz, M. J.; Eltschka, C.; Friedrich, H. *Phys. Rev. A* **2001**, 63, 042102.
  20. Friedrich, H.; Trost, J. *Phys. Rev. A* **1999**, 59, 1683.
  21. Hainz, J.; Grabert, H. *Phys. Rev. A* **1999**, 60, 1968.
  22. Flügge, S. *Practical Quantum Mechanics I*; Springer-Verlag: Berlin, 1971.
  23. Kang, J. S.; Schnitzer, H. J. *Phys. Rev. D* **1975**, 12, 841.
  24. Sergeenko, M. N. *Phys. At. Nucl.* **1993**, 56, 365.
  25. Gu, X.; Dong, S. *Phys. Lett. A* **2008**, 372, 1972.
  26. Sergeenko, M. N. *Phys. Rev. A* **1996**, 53, 6.
  27. Cooper, F.; Khare, A.; Sukhatme, U. *Phys. Rep.* **1995**, 251, 267.
  28. Yin, C.; Cao, Z. *Ann. Phys.* **2010**, 325, 528.
  29. Barclay, D. T. *Phys. Lett. A* **1994**, 185, 169.
  30. Natanzon, G. A. *Teoret. Mat. Fiz.* **1979**, 38, 146.
  31. Ginocchio, J. N. *Ann. Phys.* **1984**, 152, 203.
  32. Cooper, F.; Ginocchio, J. N. *Phys. Rev. D* **1987**, 36, 2458.
  33. Barclay, D. T.; Maxwell, C. J. *Phys. Lett. A* **1991**, 157, 357.
  34. Gedenshtein, L. *JETP Lett.* **1983**, 38, 356.
  35. Grandati, Y.; Bérard, A. *Ann. Phys.* **2010**, 325, 1235.
-