WKB approximation for analyzing quantum tunneling effect through negative Kratzer potential

Herry F. Lalus 1*, H Yudhawardana 1 and N P Aryani 2

1 Physics Department, Faculty of Teacher Training and Education, Universitas Nusa Cendana Kupang, Indonesia
2 Physics Department, Universitas Negeri Semarang, Indonesia

*Corresponding author : herrylalus@staf.undana.ac.id

Abstract. Kratzer potential is a potential for bound states in molecular bonds, while negative Kratzer potential is a potential for scattering states which has a barrier form, and which clearly has properties opposite to the bound state potential. This type of potential is the main subject of this paper. When a non-relativistic particle which has lower energy moving towards the potential, then there is a probability for the particle to break through the potential. In this paper, we use the WKB (Wenztel-Kramers-Brillouin) method to analyze the physical conditions that must be met by the system in order for the tunneling processes to occur. We present these conditions in the form of the relationship among several quantum variables such as the mass of the particle, the energy of the particle, the maximum height of the barrier potential, equilibrium internuclear separation, and the enactment domain of the potential field effect on the particle when the particle breaks through that potential.

1. Introduction

The quantum tunneling effect is a phenomenon at the molecular, atomic, or subatomic level that occurs when a particle with a certain energy \( E \) can penetrate a potential barrier \( V(r) \) with higher energy. This phenomenon does not exist in classical mechanics but occurs at the quantum level [1]. This phenomenon opened a new perspective for scientists in the 19th century so that they were able to construct quantum mechanics to become more established today. With a good understanding of the effects of this tunneling, many of the puzzles of physical phenomena begin to be answered, such as problems with radioactive decay, ionization, quantum state transitions, and so on.

The theoretical study of the tunneling effect was first carried out by Gamow in 1928 (independently of Condon and Gurney) in analyzing the alpha decay phenomenon of radioactive atomic nuclei ([1],[2]). The tunneling effect plays a very important role in physical phenomena both at the molecular, atomic, and sub-atomic levels. By knowing this mechanism, many things in the microscopic context can be known. The problem of tunneling effects also plays an important role in materials developed in the world of science to the world of industry, from research related to materials for semiconductors, superconductors, to industrial-scale materials such as graphene and optical materials ([3],[4],[5]).

Based on the medium, the tunneling effect can be divided into two, namely the linear and nonlinear tunneling effect [6–11]. The linear tunneling effect is a mechanism of the tunneling effect that occurs in the air/ vacuum medium, while the nonlinear tunneling effect, for example, is in wave propagation in non-air/ vacuum optical materials ([6],[12]). There have been many studies examining these two fields,
both linear and nonlinear ([3–6,13,14]). In terms of the analytical method, it is quite different fundamentally, which also results in the complexity of the formulation produced and then analyzed.

This research is focused on the phenomenon of the linear medium tunneling effect. More specifically, this research will focus on analyzing the quantum transmission probability (tunneling mechanism) of a charged particle passing through a potential barrier. The potential barrier to be examined in this study is a negative Kratzer potential. Kratzer potential is a type of potential that is often found in molecular interaction phenomena, and which was first introduced by Kratzer [15]. Currently, this potential study has been developed into various fields of study, for example, the quantum dot [16], statistical thermodynamics [17], the Stark effect for the bound state [16], and others [18]. Modifications to this potential can be seen in ([17,19–22]).

The Kratzer potential is basically constructed to describe the bound state of molecular interactions. One thing that is interesting is that, although Kratzer potential is a bound potential, from another point of view, this potential can be seen as a barrier for certain particles outside the system to pass through, or even by other particles in the system that tend to "break away" or change its quantum state. If another particle moves closer to that potential, that particle has the probability to penetrate or be reflected/scattered, as well as the particle which will change its quantum state (excitation), has the probability to "break away"/break through the effect of the potential in its initial state. Classically, if the energy a particle has is lower than the interaction energy of a molecule, it is impossible for the particle to penetrate that potential; but quantally, there is a probability that the particle will penetrate it.

If the system in question is molecular interactions, then basically the Kratzer potential indicates a bound state interaction, which is also a state of attraction in a molecule. However, if we are considering the possibility of transmitting other particles through molecular interactions, then the potential under review must act as a barrier/scatter potential, therefore this potential sign is made negative from the standard potential. The potential of this type ([15]) is further reviewed in this study.

This research is focused on analyzing the tunneling effect of quantum particles when they are subjected to a negative Kratzer potential. This study uses the WKB (Wentzel-Kramer-Brillouin) method in finding the probability of particle transmission. This method is one of the most powerful methods that can be used not only for solving bound states in quantum systems, but also for such unbound cases.

2. Methods
2.1. WKB approximation

In general, the WKB Method is used to solve time-independent Schrodinger equation problems that are difficult to solve/even cannot be solved exactly. This method can be applied to bound state problems (to calculate energy levels) as well as to analyze scattering phenomena (at barrier potentials) and the effect of quantum tunneling ([23–25]).

![Figure 1. A General form of Barrier Potential](image)

Since this study is focused on the tunneling effect, the description of the WKB method is only focused on this phenomenon. Before further elaborating on the WKB method, it is necessary to briefly explain the tunneling effect. This phenomenon occurs when a quantum particle penetrates through a potential barrier that has higher energy than the particle's energy. This phenomenon was first investigated by
Gamow, Gurney, and Condon to analyze radioactive decay, however, recently, the tunneling effect has been studied in many quantum areas as previously mentioned.

\[
\psi_I(x) = \frac{A}{\sqrt{k(x)}} \exp\left( i \int_a^x k(x) \, dx + \frac{\pi}{4} \right) + \frac{B}{\sqrt{k(x)}} \exp\left( -i \int_a^x k(x) \, dx + \frac{\pi}{4} \right) \tag{1}
\]

\[
\psi_{II}(x) = \frac{C}{\sqrt{k'(x)}} \exp\left( - \int_a^x k'(x) \, dx \right) + \frac{D}{\sqrt{k'(x)}} \exp\left( \int_a^x k'(x) \, dx \right) \tag{2}
\]

\[
\psi_{III}(x) = \frac{F}{\sqrt{k(x)}} \exp\left( i \int_b^x k(x) \, dx + \frac{\pi}{4} \right) \tag{3}
\]

where

\[
k(x) = \frac{\sqrt{2mE}}{\hbar}; \quad k'(x) = \frac{\sqrt{2m(V(x) - E)}}{\hbar} \tag{4}
\]

It should be remembered that the addition of the \(\pi/4\) phase in equations (1) and (3) from the actual form is solely for the purpose of facilitating the comparison of these equations with Airy function in solving the limit problem (classical turning point) to find the relationship between the constants \(F\) in region III with constant \(A\) in the region I.

If we pay attention to equation (2), there is a serious matter that must be considered, namely the amplitude part of the wave function. The factor \(\frac{1}{\sqrt{k'(x)}}\) is proportional to \(\frac{1}{\sqrt{p'(x)}}\), where \(p'(x) = \sqrt{2m(V(x) - E)}\) is the momentum of the particle in region II. However, what needs to be considered is the points \((a, E)\) and \((b, E)\), which are the classical turning points. At these two points, \(E = V(x)\), makes the factor \(\frac{1}{\sqrt{k'(x)}}\) go to infinity or the momentum factor is zero so that the wave function at this point goes to infinity. This is very contrary to experimental facts. Therefore, to solve this problem, it is necessary to connect the wave function from region I to region II, and also region II to region III.

To get the connection formula, it can be done in a few steps. First, separately observing the regions that are very close to the connection point between regions I and II, then region II and region III; this area is hereinafter referred to as the patching region. Second, the patching region is seen as a new quantum system, where the potential form is a linear potential that has a certain gradient with respect to the horizontal plane. Third, perform a solution analysis of the Schrodinger equation for this system. The solution of the Schrodinger equation system generates a patching wave function which is a linear combination of the Airy type I and type II functions. Fourth, comparing the WKB wave function for each connection area with the patching wave function corresponding to the two regions. From this relationship, the relationship between the constant \(F\) in equation (3) and the constant \(A\) in equation (1) will be obtained. This relationship is used to calculate the transmission probability \(T = \left| \frac{\psi_{II}}{\psi_I} \right|^2\). The intended Airy functions are \(Ai(w)\) and \(Bi(w)\), which generally have the form of integral representation, namely

\[
Ai(w) = \frac{1}{\pi} \int_0^\infty \cos\left( \frac{y^3}{3} + yw \right) \, dy, \tag{5}
\]

\[
Bi(w) = \frac{1}{\pi} \int_0^\infty \left( e^{-\frac{y^3}{3} + yw} + \sin\left( \frac{y^3}{3} + yw \right) \right) \, dy. \tag{6}
\]

For asymptotic condition

\[
Ai(w) \sim \frac{1}{2\sqrt{\pi w^3}} \exp\left( -\frac{2}{3} w^\frac{3}{2} \right); \quad w \gg 0, \tag{7}
\]

\[
Ai(w) \sim \frac{1}{\sqrt{\pi (-w)^3}} \sin\left( \frac{2}{3} \left( -w^\frac{3}{2} + \frac{\pi}{4} \right) \right); \quad w \ll 0 \tag{8}
\]
The first review is carried out on the right turning point, namely point \((b, E)\). The wave function for the linearized potential (patching area) in region III can be written

\[ \psi_{II-\text{p}}(w) = \eta Ai(w) + \zeta Bi(w). \]  

(11)

where

\[ w = \left( \frac{A \mu}{\hbar^2} \right) (x - x_i), \]

(12)

\( A \) is a constant, \( x_i \) is the turning point on \( x \)-axis, and \( \mu \) relates to the potential gradient. WKB wave function for region III is

\[ \psi_{III-WKB}(w) = \frac{1}{(-w)^{3/2}} \left( F e^{\frac{2}{3}(-w)^{3/2}} + G e^{-\frac{2}{3}(-w)^{3/2}} \right). \]

(13)

Based on equation (3) and (13), WKB wave function for region III can be expressed in the form

\[ \psi_{III-WKB}(w) = -F e^{\left( \frac{2}{3}(-w)^{3/2} + \frac{\pi}{4} \right)}. \]

(14)

To compare the wave functions of equations (14) and (11) which are based on Airy's function in equations (8) and (10), the form of equation (14) must be changed using Euler's formula into trigonometric form so that the form becomes

\[ \psi_{III-WKB}(w) = F \left( \cos \left( \frac{2}{3}(-w)^{3/2} + \frac{\pi}{4} \right) + i \sin \left( \frac{2}{3}(-w)^{3/2} + \frac{\pi}{4} \right) \right). \]

(15)

From equations (15) and (11), based on equations (8) and (10), we find

\[ \eta = iF \text{ \ and \ } \zeta = F. \]

(16)

Based on equation (16), it can be seen that \( \eta \) and \( \zeta \) have a relationship in the form \( \eta = i\zeta \).

Furthermore, we consider the wave function in region II (patching region) around \( x = b \), namely

\[ \psi_{II-(b)}(w) = i\zeta Ai(w) + \zeta Bi(w), \]

(17)

and WKB wave function for region II, namely

\[ \psi_{II-WKB}(w) = \frac{c}{w^{3/2}} e^{-\frac{2}{3}w^{3/2}} + \frac{d}{w^{3/2}} e^{\frac{2}{3}w^{3/2}}. \]

(18)

Then, we compare equations (17) and (18) by utilizing Airy function from equations (7) and (9), we find

\[ C = \frac{i\zeta}{2\sqrt{\pi}} = \frac{iF}{2}; \quad D = \frac{\zeta}{\sqrt{\pi} \mu} = F, \]

(19)

then

\[ \psi_{II-(b)}(x) = \left( \frac{iF}{2} \right) \frac{1}{\sqrt{k'(x)}} \left( \exp \left( - \int_b^x k'(x)dx \right) - 2i \exp \left( \int_a^x k'(x)dx \right) \right). \]

(20)

After reviewing the connection at the point \( x = b \), we continue with the connection at \( x = a \). The connection at \( x = a \) can be obtained from \( \psi_{II-(b)}(x) \) in equation (20) by changing the form of the following integral

\[ \int_a^b k'(x)dx = \int_a^x k'(x)dx + \int_a^b k'(x)dx = - \int_a^x k'(x)dx + \int_a^b k'(x)dx. \]

(21)

Using the same method as when deriving equation (20) using the form in equation (21), the wave function \( \psi_{II-(a)}(x) \) can be written
\[
\psi_{ll}^{(a)}(x) = \frac{F}{\sqrt{k'(x)}} \left( \frac{i}{2} e^{-\gamma} \exp \left( \int_{x}^{b} k'(x) dx \right) + e^{\gamma} \exp \left( - \int_{a}^{x} k'(x) dx \right) \right)
\]

where

\[
\gamma = \int_{a}^{b} k'(x) dx.
\]

Converting equation (22) into the form \(\psi(w)\) around the point \(x = a\), we get

\[
\psi_{ll-WKB}^{(a)}(w) = \frac{1}{w^{\frac{1}{2}}} \left( \frac{iF}{2} e^{-\gamma} e^{\frac{3}{2} w^{\frac{3}{2}}} + Fe^{\gamma} e^{-\frac{3}{2} w^{\frac{3}{2}}} \right).
\]

The patching wave function in the linearized potential region around \(x = a\) is

\[
\psi_{ll-\rho}^{(a)}(w) = \alpha Ai(w) + \beta Bi(w).
\]

By comparing equations (24) and (25), and utilizing Airy function in equations (7) and (9), we get

\[
\frac{\alpha}{2\sqrt{\pi}} = Fe^{\gamma} ; \quad \frac{\beta}{\sqrt{\pi}} = \frac{iFe^{-\gamma}}{2}.
\]

Next for region I, we use the form

\[
\psi_{l-WKB}(w) = \frac{1}{(-w)^{\frac{1}{2}}} \left( Ae^{i\theta} + Be^{-i\theta} \right) = \frac{1}{(-w)^{\frac{1}{2}}} \left( (A + B) \cos \theta + i(A - B) \sin \theta \right)
\]

where

\[
\theta = \frac{2}{3} (-w)^{\frac{3}{2}} + \frac{\pi}{4}.
\]

Based on equation (26), patching wave function for region I can be written

\[
\psi_{l-\rho}(w) = 2\sqrt{\pi} Fe^{\gamma} Ai(w) + \frac{i}{2} \sqrt{\pi} Fe^{-\gamma} Bi(w).
\]

Furthermore, we compare equations (27) and (29), we get

\[
A + B = 2Fe^{\gamma} ; \quad A - B = \frac{Fe^{-\gamma}}{2}.
\]

By solving equation (30), we get the relationship between \(F\) and \(A\), namely

\[
F = \frac{A e^{-\gamma}}{1 + e^{-2\gamma}}
\]

Thus, transmission coefficient \(T = \left| \frac{F}{A} \right|^{2}\), becomes

\[
T = \frac{e^{-2\gamma}}{(1 + e^{-2\gamma})^{2}}.
\]

3. Result and Discussion

3.1. Tunneling Effects through Negative Kratzer Potential

As discussed briefly in the Introduction, the Kratzer Potential is to explain the bound state of molecular interactions. The standard form of Kratzer potential is \(V(r) = -D_{e} \left( \frac{2r_{e}}{r} - \frac{r_{e}^{2}}{r^{2}} \right)\); where \(D_{e}\) is the lowest bond energy molecule, which can be viewed as the energy required to break molecular bonds/ separate molecular constituents; \(r_{e}\) is the most ideal separation distance to produce stable and strong molecular bonds; and \(r\) is the separation distance between the nuclei [18]. Based on this formula, it can be seen that \(D_{e}\) can be viewed as a potential "depth", which is also a point of vibrational equilibrium between molecules and acts as a point of bond stability.

Based on the description above, it is clear that the Kratzer potential explains the interaction of attraction between molecular constituents. Of course, this potential does not allow for quantum tunneling effects, because this potential is not in the form of a barrier potential or scatter potential. What is interesting about the potentials that explain the bonding of molecules such as the Morse Potential, Kratzer, Kratzer modification, Hellman, etc., which are in the form of potential for the bound state, but from another point of view, this potential can be seen as a barrier to certain particles outside the system
through it, or even by other particles in the system that tend to "break away" or change their quantum state [15]. When it is to be viewed in this way, the potential under review must act as a potential barrier/ scatter, therefore this potential sign is made negative from the standard potential. When made negative, then this potential form will automatically act as/ become potential with repulsive force (which will act as scatter/ barrier particles) because it will form a curve over the horizontal axis.

The form of negative Kratzer potential is

\[ V(r) = 2D_e \left( \frac{r_e}{r} - \frac{r_e^2}{r^2} \right) \]  

(33)

From equations (4) and (33), equation (23) can be written

\[ \gamma = \frac{1}{\hbar} \int_a^b \frac{\sqrt{-E r^2 + \mu_1 r + \mu_2}}{r} \, dr \]  

(34)

where \( E > 0, D_e > 0, r_e > 0, r \neq 0, \) and

\[ \mu_1 = 4mD_e r_e ; \mu_2 = -4mD_e r_e^2 ; \mu_2 = -r_e \mu_1 . \]  

(35)

From equation (35), it can be seen that \( \mu_1 > 0, \) while \( \mu_2 < 0. \) Next, equation (34) can be written

\[ \gamma = \frac{1}{\hbar} \Gamma , \]  

(36)

with

\[ \Gamma = \int_a^b \frac{\sqrt{\mu_1 r - (E r^2 + \mu_1 r_e)}}{r} \, dr , \]  

(37)

where \( \Gamma \) must be real (which is determined based on the conditions), then the solution of equation (37) for the complex solution form is expressed in the form \( \tilde{\Gamma} \). Therefore, equation (37) has an exact solution of the form

\[ \tilde{\Gamma} = H_1 + H_2 + H_3 + H_4 . \]  

(39)

where

\[ H_1 = \sqrt{\mu_1 b - (E b^2 + \mu_1 r_e)} \]  

(40)

\[ H_2 = \sqrt{\mu_1 a - (E a^2 + \mu_1 r_e)} \]  

(41)

\[ H_3 = \frac{\mu_1 i}{2 \sqrt{E}} \ln \left( \frac{a}{b} \right) \]  

(42)

\[ H_4 = i \sqrt{\mu_1 r_e} \ln \left( \frac{a}{b} \right) \]  

(43)

The first analysis carried out is to select the conditions for the real condition. From equation (40), the conditions that are met must be of the form

\[ \mu_1 b - (E b^2 + \mu_1 r_e) \geq 0 . \]  

(44)

The reason for the choice of greater is equal to zero in equation (44) because this condition is not the only condition to produce a real positive \( \gamma \) value, but it still depends on other conditions which of course can cover \( H_1 = 0 \). Thus, this particle did not deviate at all from the phenomenon being studied. Furthermore, from equation (41), the conditions that must be met are

\[ \mu_1 a - (E a^2 + \mu_1 r_e) \geq 0 . \]  

(45)
The choice of conditions in equation (45) also has the same reasons as choosing the conditions in equation (44).

Next, we analyze equation (42). This equation can be expressed in the form
\[ H_3 = \frac{\mu_1}{2\sqrt{E}} \ln \left( \frac{L_1+i2H_1}{L_2+i2H_2} \right) \quad (46) \]
where
\[ L_1 = \frac{\mu_1}{\sqrt{E}} - 2\sqrt{E}b \quad ; \quad L_2 = \frac{\mu_1}{\sqrt{E}} - 2\sqrt{E}a. \] (47)

Using the logarithmic property, equation (46) can be written in the form
\[ H_3 = \frac{\mu_1}{2\sqrt{E}} \left( \ln(L_1 i + 2H_1) - \ln(L_2 i + 2H_2) \right) \quad (48) \]
If \( \ln(L_1 i + 2H_1) \equiv \alpha_1 + \beta_1 i \) and \( \ln(L_2 i + 2H_2) \equiv \alpha_2 + \beta_2 i \), so to get real \( H_3 \), we have to choose \( \beta_1 \) and \( \beta_2 \) is negative. The conditions that must be met so that these two values are negative are \( L_1 \) and \( L_2 \) must also be negative based on equation (48). Explicitly, we have two more conditions, namely
\[ \frac{\mu_1}{\sqrt{E}} < 2\sqrt{E}b \quad ; \quad \frac{\mu_1}{\sqrt{E}} < 2\sqrt{E}a. \] (49)

So that the form used in equation (36) is in accordance with this physical state
\[ \mathfrak{R}(H_3) = \frac{\mu_1}{2\sqrt{E}} (\beta_2 - \beta_1) \] (50)
where \( \mathfrak{R}(H_3) \) is the real part of \( H_3 \). It should be noted that the conditions obtained here are still in the domain of requirements to meet the real conditions.

We now proceed to review equation (43). This equation can be expressed in the form
\[ H_4 = i\sqrt{\mu_1 r_e} \ln \left( \frac{L_3 i-2a\sqrt{r_e}H_1}{L_4 i-2b\sqrt{r_e}H_2} \right) \quad (51) \]
where
\[ L_3 = a\sqrt{\mu_1}(2r_e - b) \quad ; \quad L_4 = b\sqrt{\mu_1}(2r_e - a). \] (52)

Using the logarithmic property, equation (51) can be written as
\[ H_4 = i\sqrt{\mu_1 r_e} \left( \ln(L_3 i - 2a\sqrt{r_e}H_1) - \ln(L_4 i - 2b\sqrt{r_e}H_2) \right). \] (53)

If \( \ln(L_3 i - 2a\sqrt{r_e}H_1) \equiv \alpha_3 + \beta_3 i \) and \( \ln(L_4 i - 2b\sqrt{r_e}H_2) \equiv \alpha_4 + \beta_4 i \), so to get real \( H_4 \), we have to choose \( \beta_3 \) and \( \beta_4 \) to be negative. The conditions that must be met so that these two values are negative are \( L_3 \) and \( L_4 \) must also be negative according to equation (53). Explicitly, we have two additional conditions for reality, namely
\[ r_e < b/2 \quad ; \quad r_e < a/2. \] (54)

So that the form used in equation (36) is in accordance with this physical state
\[ \mathfrak{R}(H_4) = \sqrt{\mu_1 r_e} (\beta_4 - \beta_3) \] (55)
where \( \mathfrak{R}(H_4) \) is the real part of \( H_4 \). So the factor \( \Gamma \) has a form
\[ \Gamma = H_1 - H_2 + \mathfrak{R}(H_3) + \mathfrak{R}(H_4). \] (56)

From the analysis carried out so far, we have obtained some necessary conditions for the real state of equation (39). However, it should be noted that for the tunneling effect phenomenon, not only the real conditions of equation (39) must be met, but also the positive conditions for this equation. Therefore, the positive condition is fulfilled if \( \Gamma > 0 \), or explicitly
\[ H_1 - H_2 + \mathfrak{R}(H_3) + \mathfrak{R}(H_4) > 0. \] (57)

From equation (57), it can be seen that the combination of operations \( H_1, H_2, \mathfrak{R}(H_3), \) and \( \mathfrak{R}(H_4) \) with positive real results will allow the tunneling effect phenomenon to occur.

Based on equation (56), equation (36) can be written
\[ \gamma = \frac{1}{\hbar} \left( H_1 - H_2 + \mathfrak{R}(H_3) + \mathfrak{R}(H_4) \right). \] (58)

Furthermore, we can express equation (32) to be
\[ T = e^{-\frac{\pi}{\hbar} \left( H_1 - H_2 + \mathbb{R}(H_3) + \mathbb{R}(H_4) \right)} \cdot \frac{1}{\left( 1 + e^{-\frac{2\pi}{\hbar} \left( H_1 - H_2 + \mathbb{R}(H_3) + \mathbb{R}(H_4) \right)} \right)^\frac{\mathbb{R}}{4}}. \]  
\hspace{1cm} (59)

For cases where \( H_1 - H_2 + \mathbb{R}(H_3) + \mathbb{R}(H_4) \) is very large, then equation (59) can be written in the form

\[ T = e^{-\frac{\pi}{\hbar} \left( H_1 - H_2 + \mathbb{R}(H_3) + \mathbb{R}(H_4) \right)}. \]  
\hspace{1cm} (60)

It can be seen from equation (60) that for this situation, the WKB transmission formulation is reduced to the Gamow formula.

4. Conclusion
We have analyzed the quantum tunneling effects of particles passing through negative Kratzer potential using the WKB method. What we do is analyze the conditions that must be met for this phenomenon to occur and also compute an explicit statement of the probability of its transmission. We have presented the terms in detail at the top and specifically, the calculation of the transmission probability can be seen in equation (59). It can be seen that, when \( H_1 - H_2 + \mathbb{R}(H_3) + \mathbb{R}(H_4) \) is very large, then the transmission probability is reduced to the Gamow formula.

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