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Approximation Rectangular Function as Potential Barrier

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Abstract. Quantum tunneling occurs in the isomerization of hydroxymethylene into formaldehyde. Experiments and theory have proven the occurrence of it but both of them have a different result of the half-life of 0.7 hours. The differences the result is the motivation in this study. In theoretical, the probability of quantum tunneling calculates by Wentzel, Kreamer, Berlioun (WKB) approximation. This study calculates probability quantum tunneling use WKB and rectangular function approximation. The calculation of quantum tunneling probability with rectangular function approximation started at 1, 3, 5, 7 until 59 rectangular functions potential barrier use transfer matrix method to simplify the calculation. We use Gaussian function as the potential barrier that the height and width of the potential barrier satisfy the character of the potential barrier in isomerization hydroxymethylene barrier to formaldehyde. And the result, we get the minimum number of rectangular potential barrier to obtain a stable quantum tunneling probability value of 35 potential.

1. Introduction

The potential fields affect the movement of particles. As a result, the particle is bounding or scattering state. The bound state occurs when the particle energy is lower than the current potential of $x \to -\infty$ and $x \to \infty$. Which, the particle will trap in potential and cannot get out from the potential. Then, the scattered state occurs when the particle energy is higher than the potential barrier when $x \to -\infty$ and/or $x \to \infty$ In this state the particles can pass through the potential.

Particle in the bound state can be through the potential barrier, it is quantum tunneling. Quantum tunneling occurs in the case of isomerization of hydroxymethylene into formaldehyde. The isomerization has been proven in experiments and theoretical studies but both of them has a difference of half-life equal to 0.7 hours. Based on theoretical studies, quantum tunneling probability calculations use techniques Wentzel, Kramers, Brillouin (WKB). Another technique can use calculate quantum tunneling probability is approximation delta Dirac approximation. The previous studies, approximation delta Dirac functions have a significant result with WKB approximation. These studies calculate the probability of quantum tunneling

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2. Mathematical Method

We use Gaussian function as potential barrier. The Gaussian function satisfy the high and width from potential barrier of isomerization hydroxymethylene into formaldehyde. We approximate the potential barrier with rectangular function see Figure 2. We calculate probability quantum tunneling with matrix transfer method. The formula probability of quantum tunneling use matrix transfer method is

$$T = \left| \frac{\det \mathbf{M}}{M_{22}} \right|^2 . \tag{1}$$

T,$\mathbf{M}$, dan M_{22} respectively probability of quantum tunneling, total of matrix transfer, and a component of total matrix transfer. Total matrix transfer is

$$\mathbf{M}_n = \mathbf{M}_{n+1}.\mathbf{M}_n.\mathbf{M}_{n-1}.\mathbf{M}_{n-2}.\mathbf{M}_{n-3} \ldots \mathbf{M}_1. \tag{2}$$

From Equation 2 has three matrix transfer patterns for the beginning, middle, and final. There are

Part of Beginning

$$\mathbf{M}_{n+1} = \frac{1}{2} \begin{pmatrix} \exp[x_{n+1}(l_1 - ik)] \left(1 + \frac{l_1}{ik}\right) & \exp[x_{n+1}(-l_1 - ik)] \left(1 - \frac{l_1}{ik}\right) \\ \exp[x_{n+1}(l_1 + ik)] \left(1 - \frac{l_1}{ik}\right) & \exp[x_{n+1}(-l_1 + ik)] \left(1 + \frac{l_1}{ik}\right) \end{pmatrix}, \tag{3}$$

Part of Middle

$$\mathbf{M}_n = \frac{1}{2} \begin{pmatrix} \exp\left[x_n(l_n - l_{n-1})\right] \left(1 + \frac{l_n}{l_{n-1}}\right) & \exp\left[x_n(-l_n - l_{n-1})\right] \left(1 - \frac{l_n}{l_{n-1}}\right) \\ \exp\left[x_n(l_n + l_{n-1}1)\right] \left(1 - \frac{l_n}{l_{n-1}}\right) & \exp\left[x_n(-l_n + l_{n-1})\right] \left(1 + \frac{l_n}{l_{n-1}}\right) \end{pmatrix}, \tag{4}$$

Part of Final

$$\mathbf{M}_1 = \frac{1}{2} \begin{pmatrix} \exp[x_1(ik - l_1)] \left(1 + \frac{ik}{l_1}\right) & \exp[x_1(-ik - l_1)] \left(1 - \frac{ik}{l_1}\right) \\ \exp[x_1(ik + l_1)] \left(1 - \frac{ik}{l_1}\right) & \exp[x_1(-ik + l_1)] \left(1 + \frac{ik}{l_1}\right) \end{pmatrix}. \tag{5}$$

with,

$$x_{n+1} = a \tag{6}$$

$$x_n = x_{n+1} - \frac{2 \times a}{n} \tag{7}$$

$$x_1 = -a. \tag{8}$$

x is position of rectangular function. Then, the another component from matrix transfer are

$$l_1 = \frac{\sqrt{2m(V_1 - E)}}{\hbar}, \tag{9}$$

$$l_n = \frac{\sqrt{2m(V_n - E)}}{\hbar}, \tag{10}$$

$$l_{n-1} = \frac{\sqrt{2m(V_{n-1} - E)}}{\hbar}, \text{and} \tag{11}$$

$$k = \frac{\sqrt{2mE}}{\hbar}. \tag{12}$$

The symbol of m, V, and E sequentially is mass of particle that move position, the potential, and energy of particle.

We also calculate probability of quantum tunneling use WKB approximation.

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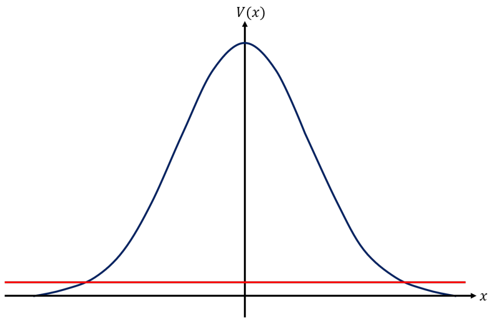

Figure 1. Potential barrier model

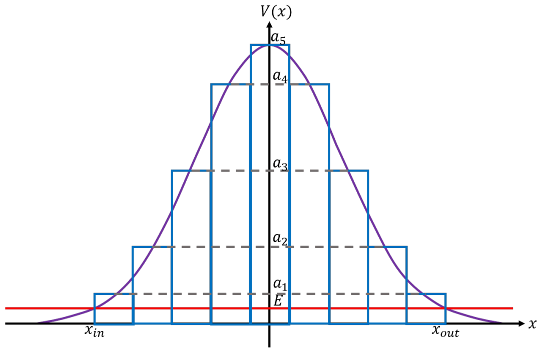

Figure 2. potential barrier model that is approached by rectangular functions

3. Result and Disscusion

We use Gaussian function as potential barrier that has high and width as 1.37 eV and 2.1 $Bohr\sqrt{amu}$. Mathematically, we formulate the Gaussian function follow :

$$V(x) = 1.37 \exp[-2.63x^2]. \tag{13}$$

The results of quantum tunneling probability use rectangular function approximation in Figure 3. From the result gave the pattern as a function. The pattern following as

$$y(x) = 1.630 \times 10^{-15} - 1.541 \times 10^{-15} \exp[-0.166x]. \tag{14}$$

It makes the result consequences follow from $\exp[x]$. The quantum tunneling probabilities will be constant starting from a point. The point is 35. That is adding 35 potential barriers rectangular function to calculate the quantum tunneling probability is starting to be constant.

The result of quantum tunneling probability use WKB approximation is 6.23×10^{-16}. This result different 4.32×10^{-17}. The differences because of the different potential barrier.

The quantum tunneling probability calculation with the rectangular function and the delta Dirac approximation has a different result. However, the quantum tunneling results with an approach rectangular functions are closer to the results of the WKB approach than the results of the quantum tunneling probability using the delta Dirac approach. That matter caused by the calculation ignoring the effects of infinite reflection of particles. The results of the quantum tunneling probability obtained with the rectangular function approach can approach the WKB result if the function with the rectangular function is minimized. However, the width of the rectangular function cannot be zero

4. Conclusion

Quantum tunneling probability calculation with rectangular function approximation start from one, three, five, seven, up to fifty-nine potential barrier rectangular function. The quantum tunneling probability is stable at a minimum number of 35 potential barrier rectangular functions. Calculation results of quantum tunneling probability with an approach box function is better than the delta Dirac approach. This is evidenced by the results of quantum tunneling probability calculations with the box function approach differs 1×10^{-1} from the quantum tunneling probability calculation with the WKB approach. Quantum tunneling probability results obtained by the box function approach can approach the WKB results if the width of the rectangular function is reduced. However, the width of the rectangular function cannot be worth zero.

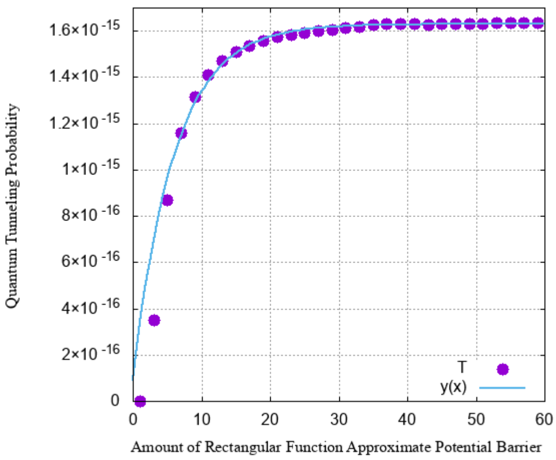

Figure 3. Graph of quantum tunneling to amount rectangular function approximate the potential barrier.

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