The Determination of the Spectrum Energy on the model of DNA-protein interactions using WKB approximation method

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Abstract. The spectrum energy’s equation for Killingbeck potential on the model of DNA and protein interactions was obtained using WKB approximation method. The Killingbeck potential was substituted into the general equation of WKB approximation method to determine the energy. The general equation required the value of critical turning point to complete the form equation. In this research, the general form of Killingbeck potential was causing the equation of critical turning point turn into cube equation. In this case we take the value of critical turning point only with the real value. In mathematical condition, it was satisfied with requirement Discriminant was less than or equal to 0. If D=0, it would give two values of critical turning point and if D<0, it would give three values of critical turning point. In this research we present both of those requirements to complete the general Equation of Energy.

1. Introduction

The molecular Interaction between DNA molecule and protein is phenomenon of utmost important for all of biological regulation. Almost all aspect of cellular function, such as transcriptional regulation chromosome maintenance, replication and DNA repair depend on the interaction of protein with DNA. DNA together with histone and non-histone proteins is the main constituent of the gene which forms the threads of chromatin then forming a chromosome [1]. At some cases, DNA-binding protein has diverse roles and functions such as making up the nucleosome, enzyme modulation chromatin structure to control the gene expression, becoming transcription factors, and as well as being cofactors. Before the DNA either replicates or transcribes, there is a certain protein which triggers the signals so that the DNA can replicate and/or transcribe, this protein is called as transcription factor [2].

All of system proses couldn’t be separated from how the DNA and protein interaction. There are many efforts to describe the model of interaction between DNA and protein. Some of them were described in 2016 by Dwiputra D et al and Syahroni E et al. [3,4]. They were described the simple model of nonlinear interaction such as the model description and stability system. In their model, Hamiltonian was used as a method to describe the total energy of the system [5]. Consider an object an atom, molecule and rock, in mechanically stable state and well isolated from its surroundings. In classical or quantum theory the object has a definite energy, which is conserved. In mechanics, energy can assume any value from some
minimum to the maximum allowed by stability. In quantum theory the possible values of energy are discrete, or quantized [6]. In this study we review the interaction between the proteins to DNA which is influenced by the potential Killingbeck only in the direction of one dimension [4]. We assumed the energy value of system was discrete. Several methods have been proposed to determine the wave function and energy [7]. In this paper we used WKB (Wentzel, Kramer and Brillouin) approximation method to determine the spectrum energy. This approximation could be used for the potential energy V(x) of system changed slowly at a small range [8]. WKB approximation is often used to solve problems in quantum mechanics either to determine the wave function and energy [9]. Several studies using WKB approach have been proposed [10, 11]

2. WKB Approximation Method

In this research, Killingbeck potential V(x) is potential that represented the interaction between DNA and the energy of protein represented with E. We used the WKB approximation to determine the spectrum energy from the interaction as equation [8]:

$$\int_{a}^{b} k(x)dx = (n + \frac{1}{2})\pi$$

(1)

with n=0,1,2,3,..., $k(x) = \frac{1}{\hbar} \sqrt{2m(E - V(x))}$, a and b are classical turning point, the value of a and b can be obtained with condition $E - V(x) = 0$ (a and b are the roots value of x).

The general form of Killingbeck potential given by equation [12, 13]:

$$V = -\frac{c}{x} + dx + \beta x^2$$

(2)

If we substituting Killingbeck potential eq. (2) to eq. (1) we have the equation to determine the spectrum energy as:

$$\int_{a}^{b} \left( E - \frac{c}{x} + dx - \beta x^2 \right)dx = \hbar \frac{n + \frac{1}{2}}{2\sqrt{2m}}$$

(3)

The classical turning point a and b can be obtained by the following equations:

$$x^3 + \frac{d}{\beta} x^2 - \frac{E}{\beta} x - \frac{c}{\beta} = 0$$

(4)

The eq. (4) is a cubic equation. As we know a cubic equation will give a solution with 3 kind of condition [14]. The solutions of the eq. (4) are:

$$x_i = S + T - \frac{d}{3\beta}$$

$$S = -\frac{1}{2} (S + T) - \frac{d}{3\beta} + \frac{1}{2} i\sqrt{3}(S - T)$$

$$T = -\frac{1}{2} (S + T) - \frac{d}{3\beta} - \frac{1}{2} i\sqrt{3}(S - T)$$

(5)
with:

$$Q = \frac{1}{9\beta^2} (3\beta E - d^3)$$

$$R = \frac{1}{18\beta^3} (3\beta Ed - 9c\beta^2 - d^3)$$

$$S = \frac{1}{3} \sqrt{R + \sqrt{Q^3 + R^2}}$$

$$T = \frac{1}{3} \sqrt{R - \sqrt{Q^3 + R^2}}$$

The solutions of eq. (4) will give the values of classical point. Before we obtained the value of classical point, we need to take a condition to classify how many classical points we need. The eq. (4) can be solved with three kinds of conditions. If c, d and $\beta$ are real and if discriminant $D=Q^3 + R^2$, than All roots are real and at least two roots are equal if $D=0$, one root is real and two are complex conjugate if $D>0$ and all roots are real and unequal if $D<0$. We take the condition with $D=0$ and $D>0$. Our aim is to get the real roots of x. After we set the condition of the classical point, the values can be substituting into the general solution of spectrum energy. The general solution of spectrum energy can be obtained from eq. (3) as followed:

$$\frac{(Eb^2 + cb - db^3 - \beta b^4)^3}{(cb + db^3 + 2\beta b^4)} - \frac{(Ea^2 + ca - da^3 - \beta a^4)^3}{(ca + da^3 + 2\beta a^4)} = -\frac{3}{2} \frac{\hbar}{\sqrt{2m}} (n + \frac{1}{2})\pi$$

(7)

2.1. Solution with condition $D=0$

The first condition is $D=0$. This condition will give three real roots with two roots are equal. The roots are given as:

$$x_1 = X = S + T - \frac{d}{3\beta} \quad \text{and} \quad x_{2,3} = -\frac{1}{2} (X + \frac{d}{\beta})$$

(8)

If $D=0$ than $Q^3$ will equal with $R^2$. By using the solutions of quadratic equation, we obtain the following equations of c from eq. (4) as:

$$c_1 = \frac{(9Ed\beta + 2d^3)}{27\beta^2} + 2\sqrt{d^6 + 3Ed^4\beta + 3E^2d^2\beta^2}$$

$$c_2 = \frac{(9Ed\beta + 2d^3)}{27\beta^2} - 2\sqrt{d^6 + 3Ed^4\beta + 3E^2d^2\beta^2}$$

(9)

The discriminant $D<0$ will be satisfied with condition of eq. (9). By substituting eq. (6) and (9) to eq. (8), we obtain the equation of classical points expressed as:

$$x_1 = -\frac{1}{3\beta} \left( \sqrt{20d^3 + 8\sqrt{d^6 + 3Ed^4\beta + 3E^2d^2\beta^2}} + d \right)$$

$$x_{2,3} = \frac{1}{6\beta} \left( \sqrt{20d^3 + 8\sqrt{d^6 + 3Ed^4\beta + 3E^2d^2\beta^2}} - d \right)$$

(10)

or

$$x_1 = -\frac{1}{3\beta} \left( \sqrt{20d^3 - 8\sqrt{d^6 + 3Ed^4\beta + 3E^2d^2\beta^2}} + d \right)$$

$$x_{2,3} = \frac{1}{6\beta} \left( \sqrt{20d^3 - 8\sqrt{d^6 + 3Ed^4\beta + 3E^2d^2\beta^2}} - 2d \right)$$

(11)

These results give two variation of classical turning point. The eq. (10) is conditions obtained with $c_1$ and eq. (11) is conditions obtained with $c_2$. 

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2.2. Solution with condition $D<0$

The second condition is $D<0$. This condition will give three real roots and all roots are unequal. If $D<0$, computation is simplified by use of trigonometry. The roots are given as:

$$\begin{align*}
    x_1 &= 2\sqrt{-Q} \cos\left(\frac{1}{3} \theta\right) - \frac{1}{3} A \\
    x_2 &= 2\sqrt{-Q} \cos\left(\frac{1}{3} \theta + 120^\circ\right) - \frac{1}{3} A \\
    x_3 &= 2\sqrt{-Q} \cos\left(\frac{1}{3} \theta + 240^\circ\right) - \frac{1}{3} A
\end{align*}$$

(12)

With $\cos \theta = \frac{R}{\sqrt{-Q}}$ or $\theta = \arccos\left(\frac{R}{\sqrt{-Q}}\right)$. If $D<0$ than $Q^3 + R^2 < 0$, by using the solutions of quadratic equation, we obtain the following equations of $c$ as:

$$\begin{align*}
    c_2 > \frac{(9Ed\beta + 2d^3) + 2\sqrt{d^6 + 3^2 Ed^5 \beta + 3^3 E^2 \beta^3 + 3^4 E^3 d^2 \beta^2}}{27 \beta^2} \\
    c_2 > \frac{(9Ed\beta + 2d^3) - 2\sqrt{d^6 + 3^2 Ed^5 \beta + 3^3 E^2 \beta^3 + 3^4 E^3 d^2 \beta^2}}{27 \beta^2}
\end{align*}$$

(13)

The discriminant $D<0$ will be satisfied with condition of eq. (13). By substituting eq. (6) to eq. (12), we obtain the equation of classical points expressed as:

$$\begin{align*}
    x_i = \frac{2}{3\beta} \left[ \sqrt{(d^2 - 3\beta E) \cos\left(\frac{1}{3} \theta\right) - 1} \right] \cdot \\
    x_i = \frac{2}{3\beta} \left[ \sqrt{(d^2 - 3\beta E) \cos\left(\frac{1}{3} \theta + 120^\circ\right) - 1} \right] \cdot \\
    x_i = \frac{2}{3\beta} \left[ \sqrt{(d^2 - 3\beta E) \cos\left(\frac{1}{3} \theta + 240^\circ\right) - 1} \right]
\end{align*}$$

(14)

3. Result and Discussion

In this section, we discuss several obtained in the previous section. The result differentiated based on the value of discriminant. Each condition of discriminant requires a condition that must be satisfied.

3.1. Condition $D=0$

By substituting the classical turning point for each condition $c_1$ and $c_2$, from eq. (10) and (11) to eq. (7), we obtain the equation to determine the energy. We use the value of each parameter as $\hbar = 1.0546$, $d = 3$, $\beta = -2$ for condition $c_1$ and $\beta = 2$ for condition $c_2$. The value of energy listed in Table 1. By inspecting Table 1, show that increase of value $n$ give different change of energies value. Both condition gives regular value of energy. In this case we take the condition with $c_2$ that corresponding to condition of a particle-bound, as electrons bound to nucleus. The energy turned toward positive corresponding with quantum state $n$. 


Table 1. Energy values corresponding to several state \( n \) of molecule DNA under the influence of Killingbeck potential with condition \( c_1 \) and \( c_2 \).

| \( n \) | \( c_1 (\beta = -2) \) | \( c_2 (\beta = 2) \) |
|-------|----------------|----------------|
| 0     | -0.0640        | 0.1053         |
| 1     | -0.0962        | 0.1898         |
| 2     | -0.1150        | 0.2093         |
| 3     | -0.1259        | 0.2161         |
| 4     | -0.1328        | 0.2191         |
| 5     | -0.1375        | 0.2206         |
| 6     | -0.1410        | 0.2216         |
| 7     | -0.1436        | 0.2222         |

In this section, we also investigate the energy value for variation of linear potential’s parameter and coupling potential’s parameter. In Table 2 shown the energy values corresponding to several variations of linear potential’s parameter \( d \) and the energy values corresponding to several variation of coupling potential’s parameter \( \beta \).

Table 2. Energy values corresponding to several state \( n \) of molecule DNA under the influence of Killingbeck potential with variation of linear parameter \( d \) and coupling parameter \( \beta \).

| \( n \) | \( d=3 \) | \( d=4 \) | \( d=5 \) | \( \beta = 2 \) | \( \beta = 3 \) | \( \beta = 3.5 \) |
|-------|---------|---------|---------|-------------|-------------|-------------|
| 0     | 0.1053  | -4.2571 | -6.6787 | -4.2571     | 0.0206      | 0.0111      |
| 1     | 0.1899  | 0.2684  | 0.3118  | 0.2683      | 0.0372      | 0.0174      |
| 2     | 0.2094  | 0.3314  | 0.4338  | 0.3314      | 0.0407      | 0.0185      |
| 3     | 0.2161  | 0.3589  | 0.4999  | 0.3589      | 0.0418      | 0.0189      |
| 4     | 0.2191  | 0.3728  | 0.5381  | 0.3728      | 0.0424      | 0.0190      |
| 5     | 0.2207  | 0.3805  | 0.5615  | 0.3805      | 0.0426      | 0.0191      |
| 6     | 0.2216  | 0.3853  | 0.5766  | 0.3853      | 0.0428      | 0.0191      |
| 7     | 0.2222  | 0.3884  | 0.5868  | 0.3883      | 0.0429      | 0.0192      |

By inspecting Table 2, show that correlation between increasing the value of each parameter. by increasing the linear potential’s parameter increase the range interval of energy value, whereas increasing the coupling potential’s parameter causing the range interval of energy become smaller.

3.2. Condition \( D<0 \)

For condition discriminant \( D<0 \), by substituting the classical turning point for each condition \( c_1 \) and \( c_2 \), from eq. (14) to eq. (7), we obtain the equation to determine the energy. With similar value of each parameter we obtained the value of energy as Table 4. Both of each condition gives a regulars value of energy. In this case we take the condition with \( c_1 \) that corresponding to condition of a particle-bound, as electrons bound to nucleus. The energy turned toward positive corresponding with quantum state \( n \).
Table 3. Energy values corresponding to several state $n$ of molecule DNA under the influence of Killingbeck potential with condition $c_1$ and $c_2$.

| $n$ | $c_1 (\beta =-2)$ | $c_2 (\beta =2)$ |
|-----|-------------------|-------------------|
| 0   | -5513.0877        | 5439.1151         |
| 1   | -5512.8399        | 5438.8722         |
| 2   | -5512.5920        | 5438.6294         |
| 3   | -5512.3442        | 5438.3866         |
| 4   | -5512.0963        | 5438.1438         |
| 5   | -5511.8485        | 5437.9009         |
| 6   | -5511.6006        | 5437.6581         |
| 7   | -5511.3527        | 5437.4153         |

We also investigate the value of energy corresponding with variation of linear potential’s parameter and coupling potential’s parameter shown in Table 4.

Table 4. Energy values corresponding to several state $n$ of molecule DNA under the influence of Killingbeck potential with variation of linear parameter $d$ and coupling parameter $\beta$.

| $n$ | $d=2$ | $d=3$ | $d=4$ | $\beta =-2$ | $\beta =-3$ | $\beta =-4$ |
|-----|-------|-------|-------|-------------|-------------|-------------|
| 0   | -5487.2644 | -5513.0877 | -5690.5127 | -5487.2644 | -2579.7821 | -1564.6055 |
| 1   | -5487.0134 | -5512.8399 | -5690.1979 | -5487.0134 | -2579.6888 | -1564.5564 |
| 2   | -5486.7625 | -5512.5920 | -5689.9201 | -5486.7625 | -2579.5956 | -1564.5073 |
| 3   | -5486.5115 | -5512.3442 | -5689.6442 | -5486.5115 | -2579.5023 | -1564.4582 |
| 4   | -5486.2605 | -5512.0963 | -5688.3067 | -5486.2605 | -2579.4090 | -1564.4092 |
| 5   | -5486.0095 | -5511.8485 | -5688.0162 | -5486.0095 | -2579.3158 | -1564.3601 |
| 6   | -5485.7585 | -5511.6006 | -5687.7035 | -5485.7585 | -2579.2225 | -1564.3110 |
| 7   | -5485.5075 | -5511.3527 | -5687.4713 | -5485.5075 | -2579.1292 | -1564.2619 |

4. Concluding remarks

In this paper, we have determined the spectrum energy for a model of a nonlinear DNA-protein interaction system with Killingbeck potential. We used the WKB approximation to determine the spectrum energy of interaction. The form of Killingbeck potential allows the energy values divided into two specific conditions. Such as with the value of discriminant $D=0$ and $D<0$. Each condition required a specific condition to satisfy. The result has shown for each condition, the value of coupling potential’s parameter $\beta$ was decisive to satisfying the condition. For $D=0$ required the value of $\beta$ greater than 0, whereas for $D<0$ required the value of $\beta$ lower than 0.

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References

[1] Bulyk M L, Gentalen E, Lockhart D J and Church G M, 1999 Nat Biotechnology 17 573–577
[2] Brivanlou A H and Darnell Jr J E 2002 Signal Transduction and Control of Gene Expression science’s Compass Review 295 813-818
[3] Dwiputra D, Hidayat W, Khairani R and Zen F P, 2016 J. phyc 694 012076
[4] Syahroni E, Suparmi A, Cari C and Fuad A, 2016 A model of a nonlinear DNA-protein interaction system with Killingbeck potential and its stability (unpublished) Submitted at the 8th International Conference on Physics and Its Applications
[5] Greiner W, 2000 Relativistic Quantum Mechanics (New York Verlag Berlin Heidelberg: Springer).
[6] Peebles P J E, 1992 Quantum Mechanic (United Kingdom: Princeton University Press) p 17
[7] Suparm A, Cari C and Deta U A, 2014 Chin. Phys. B 23 090304
[8] Suparmi, 2011mekanika Kuantum II (Surakarta : Sebelas Maret University) p 67-86
[9] Cari, Suparmi and Marini H, 2012 Indonesian journal of Applied Physics 2 112
[10] Morsche O, Sorokin S V and Peake N, 2016 J. Sound and Vibration 375 162-186
[11] Cheng K M, Leung P T and Pang C S, 2003 J. phyc. A 36. 5044-5060
[12] Killingbeck J, 1978 Phys. Lett. A 65 87
[13] Plante G and Antippa A F, 2005 J. Math. Phys. 46 062108
[14] Spiegel R M, Lipschutz and Lui J, 2009 mathematical Handbook of Formulas and Tables Third edition (USA:McGraw-Hill) p 13

Note: dirac equation jurnal scarf and new coupling tensor