Two Notes on the Theoretical Physics of ATP Synthase

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Abstract

ATP Synthase is an essential molecule in cell and molecular biology. It is responsible for the production of ATP during cellular respiration, a molecule that provides the energy required to drive a number of cellular processes. In this paper, I explore the rotational physics of ATP Synthase's rotor, a part of the protein that spins during the production of ATP. Firstly, I discuss some elementary rotational kinematics of the rotor. I then derive two alternate formulations for the total linear acceleration of the rotor. Finally, I derive formulas for the moment of inertia, angular momentum, net torque, and kinetic energy of the rotor. Through this, I hope to provide a theoretical and mathematical insight into the mechanics of ATP Synthase during the production of ATP.

1 Introduction

ATP Synthase is an essential protein to the cell. During cellular respiration, ATP Synthase is responsible for producing molecules of ATP from the hydrogen gradient established by the electron-transport chain ([1–3]). Figure 1 marks a basic picture for the structure of ATP Synthase.
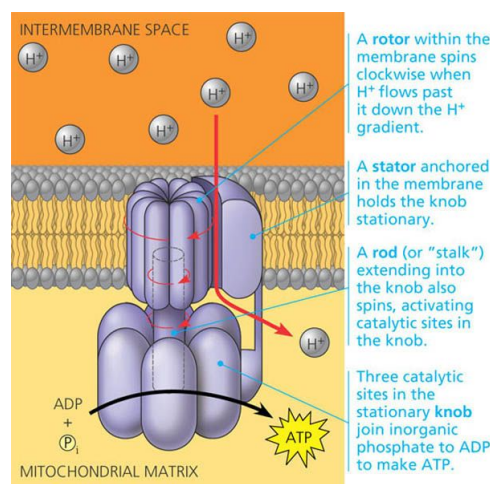

Figure 1: Comprehensive Diagram for the Structure of ATP Synthase. Taken from [3].

From figure 1, it can be seen that ATP Synthase has a rotor that spins during the mechanism of the protein, and a stator that holds the catalytic knob stationary. Furthermore, a rod that extends into the catalytic knob also spins, activating three catalytic

sites in the knob. It is at the catalytic knob where ADP is phosphorylated with inorganic phosphate to form ATP. It can also be seen from the figure that the spinning mechanism of the rotor depends on the influx of H^+ from the inter-membrane space to the mitochondrial matrix. In this paper, it is of interest to elucidate the physics of the rotor. Since the rotor spins, it is therefore of interest to explore the rotational mechanics of the rotor. Previous studies have shown that certain aspects of the rotational mechanics of the rotor are essential to the mechanism of ATP Synthase to produce molecules of ATP ([4–6]). Some of such aspects include the angular velocity, angular momentum, and torque of the rotor. In this paper, I provide mathematical formulations for a number of concepts regarding the rotational physics of the rotor. This includes the angular velocity, angular acceleration, total linear acceleration, moment of inertia, angular momentum, torque, rotational force/angle, and the rotational kinetic energy of the rotor.

2   Elementary Rotational Kinematics of the Rotor

As discussed, in order for ATP Synthase to produce ATP, the rotor must spin constantly. Since the rotor spins, it is constantly in rotational motion. Therefore, the rotational kinematics of the rotor are of interest here, and can be derived using the mathematical methods in rotational mechanics ([7–10]). Suppose that the rotor covers a displacement of 2π radians in a matter of a time t_{rev}. From this, the angular velocity of the rotor is given to be:

$$\omega_{rotor} = \frac{2\pi}{t_{rev}} \tag{1}$$

Now suppose that during a time t_{acc}, the rotor changes its angular velocity by a certain amount. This therefore results in the angular acceleration of the rotor. Letting α_{rotor} denote the angular acceleration of the rotor gives:

$$\alpha_{rotor} = \frac{\Delta\omega_{rotor}}{t_{acc}} \tag{2}$$

Letting t_{rev_i} denote the initial time it takes for the rotor to make one revolution (2π radians), and t_{rev_f} denote the final time it takes for the rotor to make one revolution, the angular acceleration of the rotor can also be denoted as:

$$\alpha_{rotor} = \frac{\frac{2\pi}{t_{rev_f}} - \frac{2\pi}{t_{rev_i}}}{t_{acc}} \tag{3}$$

Simplifying this further yields:

$$\alpha_{rotor} = \frac{2\pi}{t_{acc}} \left(\frac{1}{t_{rev_f}} - \frac{1}{t_{rev_i}} \right) \tag{4}$$

From the angular velocity, the tangential velocity v_{rotor} can be found. Assuming that a cross-section of the rotor is circular in shape, letting r_{rotor} denote the radius of the rotor gives its tangential velocity to be:

$$v_{rotor} = (r_{rotor})(\omega_{rotor}) \tag{5}$$

Furthermore, the tangential acceleration a_{rotor} is given to be:

$$a_{rotor} = (r_{rotor})(\alpha_{rotor}) \tag{6}$$

From equations 2 and 4, equation 6 can be rewritten as:

$$a_{rotor} = \frac{(r_{rotor})(\Delta\omega_{rotor})}{t_{acc}}, \tag{7}$$

and can also be rewritten as:

$$a_{rotor} = \frac{2\pi r_{rotor}}{t_{acc}}\left(\frac{1}{t_{rev_f}} - \frac{1}{t_{rev_i}}\right) \tag{8}$$

From this, the total linear acceleration of the rotor can be found. Letting $a_{T_{rotor}}$ denote this quantity, the total linear acceleration of the rotor is given to be:

$$a_{T_{rotor}} = \sqrt{a_{rotor}^2 + c_{rotor}^2}, \tag{9}$$

where c_{rotor} denotes the centripetal acceleration of the rotor. Equation 5 gives the tangential velocity of the rotor, and therefore, the centripetal acceleration of the rotor is given to be:

$$c_{rotor} = \frac{v_{rotor}^2}{r_{rotor}} \tag{10}$$

$$= r_{rotor}\omega_{rotor_i}^2 \tag{11}$$

It should be noted that ω_{rotor_i} denotes the initial angular velocity of the rotor, before the angular acceleration occurs. Firstly, using equation 7, equation 9 can be rewritten as:

$$a_{T_{rotor}} = \sqrt{\frac{r^2\Delta\omega_{rotor}^2}{t_{acc}^2} + r_{rotor}^2\omega_{rotor_i}^4} \tag{12}$$

Simplifying this further gives:

$$a_{T_{rotor}} = \sqrt{\frac{r_{rotor}^2\Delta\omega_{rotor}^2 + r_{rotor}^2\omega_{rotor_i}^4 t_{acc}^2}{t_{acc}^2}} \tag{13}$$

Taking out an r_{rotor}^2 and t_{acc}^2 gives:

$$a_{T_{rotor}} = \sqrt{\frac{r_{rotor}^2}{t_{acc}^2}\left(\Delta\omega_{rotor}^2 + \omega_{rotor_i}^4 t_{acc}^2\right)} \tag{14}$$

Which finally gives the total linear acceleration to be:

$$a_{T_{rotor}} = \frac{r_{rotor}}{t_{acc}}\sqrt{\Delta\omega_{rotor}^2 + \omega_{rotor_i}^4 t_{acc}^2} \tag{15}$$

Figure 2 renders a plot relating the change in angular velocity and total linear acceleration in equation 15 when the rotor begins rotating from rest.

Next, using equation 8, equation 9 can also be rewritten as:

$$a_{T_{rotor}} = \sqrt{\frac{4\pi^2 r_{rotor}^2}{t_{acc}^2}\left(\frac{1}{t_{rev_f}} - \frac{1}{t_{rev_i}}\right)^2 + r_{rotor}^2\omega_{rotor_i}^4} \tag{16}$$

Simplifying further then gives:

$$a_{T_{rotor}} = \sqrt{\frac{4\pi^2 r_{rotor}^2\left(\frac{1}{t_{rev_f}} - \frac{1}{t_{rev_i}}\right)^2 + r_{rotor}^2\omega_{rotor_i}^4 t_{acc}^2}{t_{acc}^2}} \tag{17}$$

Taking out an r_{rotor}^2 and t_{acc}^2 again gives:

$$a_{T_{rotor}} = \sqrt{\frac{r_{rotor}^2}{t_{acc}^2}\left[4\pi^2\left(\frac{1}{t_{rev_f}} - \frac{1}{t_{rev_i}}\right)^2 + \omega_{rotor_i}^4 t_{acc}^2\right]}, \tag{18}$$

which finally gives our alternative formula for the total linear acceleration of the rotor to be:

$$a_{T_{rotor}} = \frac{r_{rotor}}{t_{acc}}\sqrt{4\pi^2\left(\frac{1}{t_{rev_f}} - \frac{1}{t_{rev_i}}\right)^2 + \omega_{rotor_i}^4 t_{acc}^2} \tag{19}$$

Next, I formulate mathematical equations for the angular momentum and net torque of the rotor.
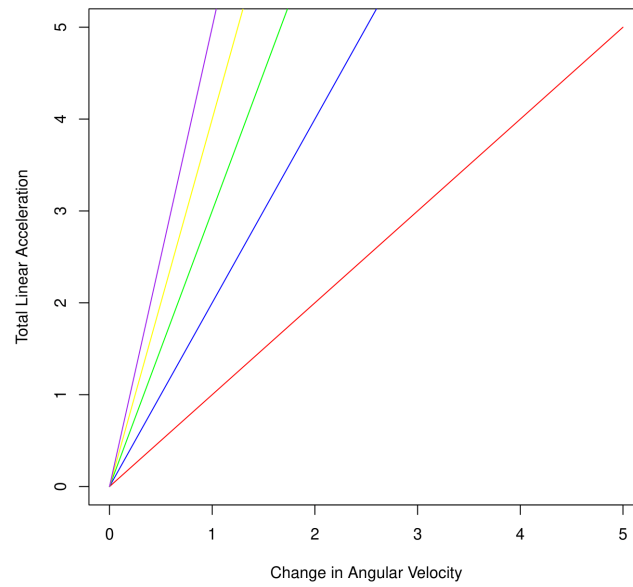
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Figure 2: Relationship between $\Delta\omega_{rotor}$ and $a_{T_{rotor}}$ when the rotor spins from rest. As it can be seen, both variables render a linear relationship, where the slope is r_{rotor}/t_{acc}. The graph displays the relationship between the two variable for $r_{rotor}/t_{acc} = 1, 2, 3, 4, 5$.

3   Moment of Inertia, Angular Momentum, Torque, and Kinetic Energy of the Rotor

Since the rotor is in rotational motion, it also possesses angular momentum. However, before discussing angular momentum, it would be of interest to find the moment of inertia of the rotor. Assume that the rotor is a solid cylinder rotating about its central axis. Letting m_{rotor} denote the rotor's mass, the moment of inertia I_{rotor} of the rotor is given to be:

$$I_{rotor} = \frac{1}{2}(m_{rotor})(r_{rotor})^2 \tag{20}$$

From this, the angular momentum of the rotor can be found. Letting ω_{rotor} denote the angular velocity of the rotor as before, the angular momentum L_{rotor} of the rotor can be denoted:

$$L_{rotor} = (I_{rotor})(\omega_{rotor}) \tag{21}$$

$$= \frac{1}{2}(m_{rotor})(r_{rotor})^2(\omega_{rotor}) \tag{22}$$

Now suppose that during a time t_{tor}, the angular momentum of the rotor changes, due to a change in the angular velocity of the rotor. Due to this change in angular momentum, a net torque acts on the rotor. Letting τ_{net} denote the net torque of the rotor, the net torque of the rotor is written as:

$$\tau_{net} = \frac{\Delta L_{rotor}}{t_{tor}} \tag{23}$$

Using our result from equation 22, the net torque can be written as:

$$\tau_{net} = \frac{(m_{rotor})(r_{rotor})^2(\Delta\omega_{rotor})}{2t_{tor}} \tag{24}$$

From this, letting F_{rotor} denote a force acting on the rotor that causes its rotational motion, and letting θ denote the angle at which the force is applied to the rotor, from

equation 24, it can be equated:

$$(r_{rotor})(F_{rotor})(\sin(\theta)) = \frac{(m_{rotor})(r_{rotor})^2(\Delta\omega_{rotor})}{2t_{tor}} \tag{25}$$

Cancelling out r_{rotor} from both sides of the equation yields:

$$(F_{rotor})(\sin(\theta)) = \frac{(m_{rotor})(r_{rotor})(\Delta\omega_{rotor})}{2t_{tor}} \tag{26}$$

From this, the value of F_{rotor} can be found using the following relation:

$$F_{rotor} = \frac{(m_{rotor})(r_{rotor})(\Delta\omega_{rotor})}{2t_{tor}(\sin(\theta))}, \tag{27}$$

and the value of θ can be found as:

$$\theta = \sin^{-1}\left(\frac{(m_{rotor})(r_{rotor})(\Delta\omega_{rotor})}{2t_{tor}(F_{rotor})}\right) \tag{28}$$

The value of the final velocity after a change in angular momentum can be found using the initial and final moment of inertias of the rotor, based on the law of conservation of angular momentum. Letting I_{rotor_i} and I_{rotor_f} denote these moment of inertias, and letting ω_{rotor_i} and ω_{rotor_f} denote the initial and final angular velocities of the rotor, it can be written:

$$\omega_{rotor_f} = \frac{I_{rotor_i}}{I_{rotor_f}}\omega_{rotor_i} \tag{29}$$

Finally, it would be of interest to determine the kinetic energy of the rotor for a certain angular velocity. The kinetic energy K_{rotor} of the rotor can be written as:

$$K_{rotor} = \frac{1}{2}(I_{rotor})(\omega_{rotor})^2 \tag{30}$$

From our result in equation 20, the kinetic energy of the rotor can be written as:

$$K_{rotor} = \frac{1}{2}(\omega_{rotor}^2)\left(\frac{1}{2}(m_{rotor})(r_{rotor})^2\right) \tag{31}$$

$$= \frac{1}{4}(m_{rotor})(r_{rotor})^2(\omega_{rotor})^2 \tag{32}$$

Figure 3 renders a plot relating the rotational kinetic energy and angular velocity discussed in equation 32.

Conclusions

In this paper, I have provided mathematical formulations for certain aspects of the rotational physics of ATP Synthase. Equation 1 provides a formula for the angular velocity of the rotor, and equations 2 and 4 provide alternative formulas for the angular acceleration of the rotor. From this, the tangential velocity and acceleration of the rotor are found in equations 5 and 6. Using these formulas, two alternative formulas for the total linear acceleration of the rotor are derived and laid out in equations 15 and 19. Then, an equation for the moment of inertia of the rotor is rendered in equation 20, and using this, a formula for the angular momentum of the rotor is found in equation 22. Based on a change in the angular momentum of the rotor, an equation for the net torque is then derived and displayed in equation 24. From the rotor's torque formula, equations for the rotational force and for the angle at which the force is applied are also derived
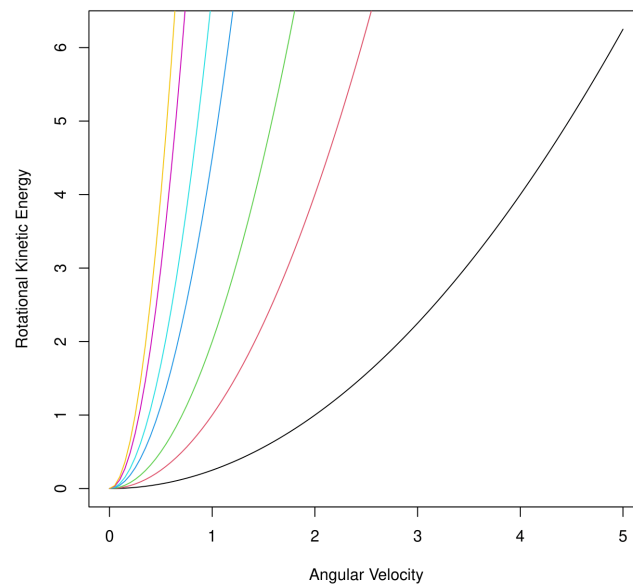
Figure 3: Curves relating the rotational kinetic energy and angular velocity of the rotor for different values of m_{rotor} and r_{rotor}. As it can be seen, K_{rotor} and ω_{rotor} render a quadratic relationship with each other.

and presented in equations 27 and 28. Finally, a formula for the rotational kinetic energy of the rotor is derived and exhibited in equation 32. Figures 2 and 3 are also laid out to provide a visual representation of the theoretical models presented in equations 15 and 32. Through this, my paper elucidates the mathematical theory behind the rotational physics of ATP Synthase, which can prove significant to further research regarding the biophysics of ATP Synthase, and therefore, of cellular respiration and ATP synthesis. Comprehensively, I hope to provide a significant insight regarding the rotational mechanics of ATP Synthase, and hope that my work can be used for future research in the fields of biophysics, biochemistry, mathematical biology, and cell/molecular biology.

4   Author Contributions

This article has been authored by AC.

5   Competing Interests

The author declares no competing interests.

6   Data Availability

The data that supports the findings of this study are available within the article.

7   Figure Legends

1. Figure 1: Comprehensive Diagram for the Structure of ATP Synthase. Taken from [3].

2. Figure 2: Relationship between $\Delta\omega_{rotor}$ and $a_{T_{rotor}}$ when the rotor spins from rest. As it can be seen, both variables render a linear relationship, where the slope is r_{rotor}/t_{acc}. The graph displays the relationship between the two variable for $r_{rotor}/t_{acc} = 1, 2, 3, 4, 5$.

3. Figure 3: Curves relating the rotational kinetic energy and angular velocity of the rotor for different values of m_{rotor} and r_{rotor}. As it can be seen, K_{rotor} and ω_{rotor} render a quadratic relationship with each other.

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