Quantum-Mechanical Brayton Engine based on a Boson Particle Inside Cubic Potential

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Abstract. Currently, the heat engine needs to be miniaturized to increase its thermal efficiency. In this theoretical study, the symmetrical potential box containing one particle with one of its walls moving freely is analogous to a cylinder with a piston. The potential box contains a massless Boson particle, while the piston-cylinder contains a monatomic ideal gas. The form of Quantum-Mechanical Brayton Engine (QMBE) thermal efficiency formulation has similarities to the classical version of the Brayton engine. However, the efficiency value of QMBE with a massless Boson particle is higher than the classic version because the heat capacity ratio of the Boson particle working fluid is 2, while the monatomic ideal gas is 5/3.

Keywords: thermal efficiency, quantum Brayton engine, heat capacity ratio, pressure ratio, compression ratio.

1. Introduction
The heat energy in the environment can be converted into work by a device called a heat engine. According to the second law of thermodynamics, a heat engine cannot convert all the absorbed heat into mechanical work, so the efficiency of a heat engine is always less than 100 percent. The efficiency $\eta$ is the ratio between the $W_{net}$ work of the engine in one cycle and the $Q_{Abs}$ heat flowing into the system. Thermal efficiency in the classical version of the engine is still considered small because not much heat is absorbed by the system and is converted to mechanical work, so the residual heat is ejected by the system and flowing into a low-temperature bath. Therefore, the system in use today is miniaturized to the quantum system to increase the efficiency of the engine.

Research on quantum heat engines began with Scovil et al [3] and Bender et al [4]. Bender et al researched the efficiency of the quantum version of the Carnot engine. This theoretical study obtaining an efficiency formulation that had the same form as the classical version of the Carnot engine [4]. Research on quantum heat engines continues today [5-11].

The quantum Brayton engine has been investigated previously by Singh [4] and Akbar [10] using a quantum system of the one-dimensional potential box containing a particle. The particle used in Singh's study was classical, while those used by Akbar was a massless Boson particle. This theoretical research offers the formulation of a Brayton engine with a quantum system, namely a cubic potential well containing a massless Boson particle.

2. The Thermal Efficiency of QMBE
The method used is an analytical method by building a physical model, then create a mathematical model that represents the physical model used. The physical model used is the quantum system which has the closest analogy to the classical version (piston-cylinder). The symmetric three-dimensional infinite potential well with one of the walls moving like a piston is the physical model used in this investigation (see Figure 1). Because the system implemented is a quantum system, several thermodynamic quantities in classical systems such as temperature (T), pressure (P), and volume (V) are converted into energy (E), force (F), and well width (L), respectively. The equation that describes the quantum system used is

$$\hat{H} \phi = -\hbar^2 c^2 \nabla^2 \phi.$$  \hspace{1cm} (1)

Eq. (1) is the Klein-Gordon equation used to describe the massless Boson particles [12]. If we apply the boundary condition $\phi(0, y, z) = \phi(L, y, z) = \phi(x, 0, z) = \phi(x, L, z) = \phi(x, y, 0) = \phi(x, y, L) = 0,$ the solution of the formulation is

$$\phi_{klm} = \frac{8}{L^3} \sin \frac{k \pi x}{L} \sin \frac{l \pi y}{L} \sin \frac{m \pi z}{L}.$$ \hspace{1cm} (2)

The energy that owned by the system is

$$E_{klm} = (k + l + m) \frac{\pi \hbar c}{L}.$$ \hspace{1cm} (3)

with quantum number $k, l, m = 1, 2, 3, \ldots$. By knowing the system energy in the Eq. (1), the mechanical force on the potential wall is

$$F_{klm} = (k + l + m) \frac{\pi \hbar c}{L^2}.$$ \hspace{1cm} (4)

To get the thermal efficiency value from QMBE, we need to know the value of the system's work in one cycle and the amount of heat that enters the system. In this theoretical research, we assume there are only two states that contribute to the wave function and energy of the system.

**Figure 1.** The symmetrical potential box containing a massless Boson particle

**Figure 2.** The QMBE cycle.

**Figure 2** shown the Brayton engine has four thermodynamic processes in one cycle. Each of these processes is in a quasistatic state. Because each process is quasistatic, the system conditions at each point or both points are in thermodynamic equilibrium [1]. Isobaric expansion becomes the first stage of the thermodynamic process in this study. During the process, $Q_{abs}$ heat enters from a high energy bath into the system. The incoming heat causes the excited particles from the ground state to the first excited state. Because the particle undergoes excitation, the wave function will be...
\[ \Phi_{AB} = a_{111} \phi_{111} + a_{211} \phi_{211} + a_{121} \phi_{121} + a_{112} \phi_{112}. \]  

(5)

The energy of the system is

\[ E_{AB} = \left( 4 - |a_{111}|^2 \right) \frac{\pi \hbar c}{L}. \]  

(6)

The mechanical force of the wall can be formulated by

\[ F_{AB} = \left( 4 - |a_{111}|^2 \right) \frac{\pi \hbar c}{L}. \]  

(7)

Because the process in step one is isobaric, the condition for this process is the force in a constant state \[ F_A(L_A) = F_B(L) \]. By this condition, the length of the well at point B (\( L_B \)) is

\[ L_B = L_A \sqrt{\frac{4}{3}}. \]  

(8)

By using Eq. (7) and (8), the system’s mechanical work in the first step is

\[ W_{AB} = 3 \frac{\pi \hbar c}{L} \left( \frac{4}{\sqrt{3}} - 1 \right). \]  

(9)

The amount of heat \( Q_{Abs} \) flowing from the high energy bath into the system is

\[ Q_{Abs} = 2 \frac{\pi \hbar c}{L_A} \left( \sqrt{12} - 3 \right). \]  

(10)

The system undergoes the expansion process from point B until C adiabatically at step 2. In this step, the probability of the particle that occupied an eigenstate is fixed. The particle wave function in this process is

\[ \Phi_{BC} = a_{211} \phi_{111} + a_{121} \phi_{121} + a_{112} \phi_{112}. \]  

(11)

with the energy of the system is

\[ E_{BC}(L) = 4 \frac{\pi \hbar c}{L}. \]  

(12)

The potential well walls mechanical force \( F_{BC} \) is

\[ F_{BC}(L) = 4 \frac{\pi \hbar c}{L^2}. \]  

(13)

By using Eq. (8) and (13), the mechanical work of the system in the second step is

\[ W_{BC} = 4 \pi \hbar c \left( \frac{1}{L_A} \sqrt{\frac{3}{4}} - 1 \right). \]  

(14)

The compression from point C to D isobarically is the third thermodynamic process in this cycle. The particle is de-excited from the first excitation state to the ground state due to heat energy that cannot be converted into the work to flow out of the system to the low energy reservoir. Because the particle level state is changing, the wave function will be

\[ \Phi_{CD} = \Phi_{AB} = a_{111} \phi_{111} + a_{211} \phi_{211} + a_{121} \phi_{121} + a_{112} \phi_{112}. \]  

(15)
with the system’s energy is

$$E_{CD} = \left(4 - |a_{111}|^2\right) \frac{\pi \hbar c}{L}$$

(16)

By Eq. (16), the mechanical force of the wall is

$$F_{CD} = \left(4 - |a_{111}|^2\right) \frac{\pi \hbar c}{L^2}$$

(17)

Because the process at this stage is isobaric, the condition that must be fulfilled is \([F_c(L_c) = F_{CD}(L)]\).

Under these conditions, the width of the potential well at point D (L_D) is

$$L_D = L_C \sqrt{\frac{3}{4}}$$

(18)

The mechanical work \(W_{CD}\) system at this step is

$$W_{CD} = 4 \frac{\pi \hbar c}{L_C} \left(\sqrt{\frac{3}{4}} - 1\right)$$

(19)

The last process is the compression adiabatically from point D (L_D) back to point A (L_A). The probability that a particle is in the ground state doesn't change. Therefore, the particle wave function will become

$$\phi_{DA} = \phi_{111}$$

(20)

The energy that the system has is

$$E_{DA} = 3 \frac{\pi \hbar c}{L}$$

(21)

By Eq (21), the force generated from a potential wall is

$$F_{DA} = 3 \frac{\pi \hbar c}{L^2}$$

(22)

The mechanical work of the system in the fourth step is

$$W_{DA} = 3\pi \hbar c \left(\frac{1}{L_C} \sqrt{\frac{4}{3}} - \frac{1}{L_A}\right)$$

(23)

The summation result of Eq (9), (14), (19), and (23), the total work of QMBE in one cycle is

$$W_{net} = 2\pi \hbar c \left(\sqrt{12} - \frac{3}{L_A} + \sqrt{12} - \frac{4}{L_C}\right)$$

(24)

The QMBE’s thermal efficiency based on a single massless Boson particle trapped in a symmetrical potential box using Eq (10) and (24) is

$$\eta_{3D} = 1 - \frac{4}{\sqrt{3}} \left(\frac{L_A}{L_C}\right)$$

(25)

If Eq (25) is changed in the pressure ratio, the equation will become
\[ \eta_{3D} = 1 - \left( \frac{1}{R_F} \right)^2. \]  \hspace{1cm} (26)

with \( R_F \)

\[ R_F = \frac{F_A}{F_C}. \]  \hspace{1cm} (27)

3. Result and Discussion

If we look at equations (25) and (26), the formulation of the efficiency of QMBE is the same as the classical version, which depends on the compression ratio and \( R_F \) pressure ratio [1,2]. The difference between the classical system and the quantum system is in their working substances which is shown in Table 1. The value of each work substance is different and determined by the ratio of heat capacity to constant pressure with constant volume. In addition to the pressure and compression ratio, the heat capacity ratio value of the working substance can also affect the efficiency value.

Table 1. The thermal efficiency equation form depends on the pressure ratio

| No | The system of Brayton engine | The form of the equation | Heat capacity ratio |
|----|-------------------------------|--------------------------|--------------------|
| 1  | Piston cylinder (monoatomic gas) | \( \eta_{3D} = 1 - \left( \frac{1}{R_p} \right)^{2/3} \) | 5/3 |
| 2  | Infinite potential box (nonrelativistic particle) | \( \eta_{3D} = 1 - \left( \frac{1}{R_F} \right)^{2/3} \) | 3 |
| 3  | Infinite potential box (Relativistic particle) | \( \eta_{3D} = 1 - \left( \frac{1}{R_F} \right)^{1/2} \) | 2 |

Table 2. The thermal efficiency equation form depends on the compression ratio.

| No | The system of Brayton engine | The form of the equation |
|----|-------------------------------|--------------------------|
| 1  | 1D                            | \( \eta_{1D} = 1 - \sqrt{\frac{L_A}{L_C}} \) |
| 2  | 2D                            | \( \eta_{2D} = 1 - \sqrt{\frac{3}{2}} \left( \frac{L_A}{L_C} \right) \) |
| 3  | 3D                            | \( \eta_{3D} = 1 - \sqrt{\frac{4}{3}} \left( \frac{L_A}{L_C} \right) \) |
If we substitute the same pressure ratio $R_F$ value to the three thermal efficiency equations in Table 1, the curve is shown in Figure 3(a) will be formed. The value of QMBE single massless Boson particle thermal efficiency is higher when compared to the classic version of the Brayton engine. However, this efficiency value is lower when compared to QMBE with a single nonrelativistic particle. This happens because the value of the heat capacity ratio on the QMBE contains a single nonrelativistic particle which is greater than the classical and the single relativistic particle version. Table 2 shown the form of thermal efficiency equation between 1D [10], 2D, and 3D infinite potential box. The difference between these three equations is the number of degrees of freedom. If we substituting the same value of the compression ratio to these equations, it will form a graph in Figure 3(b). The QMBE with a 3D box system has higher efficiency values than one and two dimensions. The thermal efficiency of the QMBE with a 3D box system is higher because the system has three degrees of freedom, whereas a QMBE with a 1D and 2D system has only one and two degrees of freedom, respectively.

4. Conclusion

From the result and discussion that were presented in the previous session, two things can be concluded about the efficiency of the Brayton engine. First, the thermal efficiency value of the QMBE with a relativistic particle has a higher efficiency than the classical system but lower when compared with the nonrelativistic ones in the same pressure ratio.

Second, the thermal efficiency with a 3D system has a higher value when compared to 1 and 2 dimensional well systems. The 3-dimensional potential well system has a high-efficiency value due to the number of degrees of freedom that the system has is 3, which is represented by the state level $k$, $l$, and $m$.

5. Acknowledgments

We thank the committee of the Borneo International Conference on Applied Mathematics and Engineering (BICAME 2020) for the opportunity that has been given to us to present this research and LPPM ITK for funding this research according to contract number: 2833/IT10.II/PPM.01/2020.

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