Three-State Quantum Heat Engine Based on Carnot Cycle

Trengginas E. P. Sutantyo
Nuclear and Theoretical Physics Research Group,
Department of Physics, Faculty of Mathematics and Natural Sciences, Universitas Andalas,
Kampus Unand Limau Manis, Padang, West Sumatera 25163

ABSTRACT

In this paper, we consider three models of quantum heat engines based on Carnot cycle using three energy levels: (1) the ground state, (2) the degenerate state, and (3) the highest energy state. We investigate the variation in the transition state by selecting three different degenerated states. The result we obtained still analogous with the classical heat engine efficiency and also the previous Quantum Carnot Engine model, which only depends on the initial width and the final width of the potential well in isothermal expansion. Moreover, the effect of transition state generally can be accepted for multistate quantum heat engines with 3D systems in cubic potential.

1. INTRODUCTION

Since the beginning of the quantum era, physicists have tried to find various interrelated connections between classical physics and quantum physics, including the relevance of thermodynamics and quantum. Nowadays, quantum thermodynamics has become a very active research topic, especially for the issue of Quantum Heat Engine (QHE) models (Ferdi, 2019); (Fernandez and Omar, 2019); (Singh, 2019); (Saputra and Rifani, 2019); (Akbar et al., 2018); (Setyo and Latifah, 2018); (Thomas et al., 2017); (Anders and Giovannetti, 2013); (Muñoz et al., 2012); (Latifah and Purwanto, 2011); (Quan et al., 2007); (Rezek and Kosloff, 2006). Started by the pioneers of QHE idea, Scovil and Schulz-DuBois (1959), the purpose of the quantum approach in modeling a heat engine is to discover the most efficient heat engine model. As we know the efficiency of Classical Heat Engine (CHE) restricted by the second law of thermodynamics (Callen, 1985), i.e., the ratio between absorbed heat and produced mechanical work will always less than 1

\[ \eta = \frac{W}{Q_{Abs}} < 1 \]  \hspace{1cm} (1)

In contrast with CHE, QHE produce the work by utilizing quantum effects, such as discrete energy levels, quantum coherence, or quantum confinement (Saputra and Purwanto, 2010). According to those quantum properties, physicists expect QHE will obtain a more efficient cycle than a CHE.
However, QHE also uses classical thermodynamic cycles such as Otto (Rezek and Kosloff, 2006), Brayton (Singh, 2019), and Carnot cycle (Bender et al., 2000). Bender et al. (2000) propose the theoretical QHE model based on Carnot cycle that obtains the efficiency as follow

\[ \eta = 1 - \frac{E_C}{E_H}, \]  

in which \( E_C \) and \( E_H \) are Hamiltonian expectation values that analogous with the classical quantities \( T_C \) and \( T_H \). Besides, several other analogies such as the potential well width analog to the piston volume and the force exerted by the particle follows the relation

\[ F = -\frac{dE(L)}{dL}, \] 

analogous with the pressure on the piston wall. Those analogies produce efficiencies relevant to the CHE (Bender et al., 2000); (Belfaqih et al., 2015); (Sutantyo et al., 2015). The development of Bender et al. model by using 2D (Belfaqih et al., 2015) and 3D (Sutantyo et al., 2015) system get a more efficient heat engine.

This paper will discuss a three-state quantum heat engine model based on Carnot cycle by using Sutantyo et al. (2015) formalism. This paper organized as follows: Chapter II discusses three models of Quantum Carnot Engine. We variate the transition state by selecting various degeneration states. In chapter III, we calculate the heat engine efficiency. And then in the last chapter, we discuss the comparison of QHE models with two states model and concludes the overall result according to the addition of a degenerated state.

2. **FORMALISM OF QUANTUM CARNOT ENGINE**

In this section, we will compare three heat engine models based on Carnot cycle, each model has three energy states. From the Schrödinger equation \( \hat{H} |\Psi \rangle = E |\Psi \rangle \) for a particle with mass \( m \) in a 3D cubic potential with volume \( L^3 \), we get an eigen-energy (Zettili, 2009),

\[ E_{n_x,n_y,n_z} = \frac{\pi^2 \hbar^2}{2mL^2} \left( n_x^2 + n_y^2 + n_z^2 \right) \]

The first energy level is (1) the ground state with \( n_x,n_y,n_z = (111) \). Second level (2) has three different of each model as follow; for model A with \( n_x,n_y,n_z = (211), (121), (112) \), whereas model B with \( n_x,n_y,n_z = (221), (212), (122) \), and model C with \( n_x,n_y,n_z = (311), (131), (113) \). The highest state (3) is the fourth level of excitation with \( n_x,n_y,n_z = (222) \), which will be achieved by the system when the isothermal expansion process ends. During isothermal processes, Hamiltonian expectation value remains constant. Whereas the adiabatic processes occur in the same state. We start from the ground state, with energy

\[ E_{111} = E_H = \frac{3\pi^2 \hbar^2}{2mL_1^2}. \]

By substituting (5) into (3), we have the forces on the moving-side cubic potential

\[ F_x = F_y = F_z = \frac{3\pi^2 \hbar^2}{mL_1^3}. \]

From (5) and (6), we calculate the force in every single thermodynamics process for each QHE model.
2.1 Quantum Carnot Engine Model A

In this model, the state of the system is a linear combination of ground state, first excitation state, and fourth excitation state, which is represented by

$$\Psi_{(A)} = a_{111} \psi_{111} + a_{211} \psi_{211} + a_{121} \psi_{121} + a_{112} \psi_{112} + a_{222} \psi_{222}. \quad (7)$$

By using the relation $a_{111}^2 + a_{211}^2 + a_{121}^2 + a_{112}^2 + a_{222}^2 = 1$, we simplify the Hamiltonian expectation value $E(L)$ as a function $L$, only depending on the probability constant $a_{111}$ and $a_{222}$. The first process is isothermal expansion; the system keeps the energy constant. This condition can occur only if the energy

$$E^{(A)}(L) = \frac{3\pi^2 \hbar^2}{2mL^2} \left(2 - a_{111}^2 + 2a_{222}^2\right) \quad (8)$$

same as the ground state energy in (5), so we have relations

$$L^2 = L_{(A)1}^2 \left(2 - a_{111}^2 + 2a_{222}^2\right). \quad (9)$$

We get the force on this process by using relation (3),

$$F_{1x}^{(A)}(L) = F_{1y}^{(A)}(L) = F_{1z}^{(A)}(L) = \frac{3\pi^2 \hbar^2}{mL_{(A)1}^2 L}. \quad (10)$$

After that, the particle uses this force to push the moving sides when $L_{(A)2} = 2L_{(A)1}$, when the state has reached the fourth level of excitation, $a_{111} = 0$ and $a_{222} = 1$. The Hamiltonian expectation value express as,

$$E_2^{(A)} = \frac{12\pi^2 \hbar^2}{2mL_{(A)2}^2}. \quad (11)$$

The next process is adiabatic expansion. By using energy from the eq. (11), the force of

$$F_{2x}^{(A)}(L) = F_{2y}^{(A)}(L) = F_{2z}^{(A)}(L) = \frac{12\pi^2 \hbar^2}{mL^3} \quad (12)$$

push the moving-sides of cubic potential from $L_{(A)2}$ to $L_{(A)3} = k_{(A)}L_{(A)2}$, and $k_{(A)} > 1$. Adiabatic expansion occurs in the highest state. At the end of this process, the Hamiltonian expectation value is reduced to

$$E_{c}^{(A)} = \frac{12\pi^2 \hbar^2}{2mL_{(A)3}^2}. \quad (13)$$

Then, the system isothermally compresses from $L_3$ to $L_4$. In this process, the particle deexcitates from the fourth level to the ground state. In order to keep Hamiltonian expectation value remains constant, we set (13) equal to (8), so the width relation is

$$L^2 = \frac{L_{(A)3}^2}{4} \left(2 - a_{111}^2 + 2a_{222}^2\right). \quad (14)$$

The Forces
\[ F^{(A)}_{3x}(L) = F^{(A)}_{3y}(L) = F^{(A)}_{3z}(L) = \frac{12\pi^2 h^2}{mL_{(A)4}^2 L} \] (15)

hold the wall movement until it reaches the maximum compression, \( L_{(A)4} = L_{(A)3}/2 \), when the system returns to the ground state, \( a_{111} = 1 \) and \( a_{222} = 0 \). During this process, the Hamiltonian expectation value constant at

\[ E^{(A)}_3 = E^{(A)}_C = \frac{3\pi^2 h^2}{2mL_{(A)4}^2}. \] (16)

In the last process, the system adiabatically compresses until it returns to \( L_f \). The system remains in a ground state with the Hamiltonian expectation value increasing up to

\[ E = \frac{3\pi^2 h^2}{2mL^2}, \] (17)

which is used as the initial energy of the next cycle. The force in this process is

\[ F^{(A)}_{4x}(L) = F^{(A)}_{4y}(L) = F^{(A)}_{4z}(L) = \frac{3\pi^2 h^2}{mL^2}. \] (18)

### 2.2 Quantum Carnot Engine Model B

The state of the Model B system is a linear combination of ground state, second excitation level, and fourth excitation level, which is represented by the wave function

\[ \Psi_{(b)} = a_{111}\psi_{111} + a_{221}\psi_{221} + a_{212}\psi_{212} + a_{122}\psi_{122} + a_{222}\psi_{222} \] (19)

and \( a_{111}^2 + a_{221}^2 + a_{212}^2 + a_{122}^2 + a_{222}^2 = 1 \). The formalism of model B is similar to model A. The first process is isothermal expansion. To keep the eigenvalue constant, then \( E^{(B)}(L) \),

\[ E^{(B)}(L) = \frac{3\pi^2 h^2}{2mL^2} \left( 3 - 2^2_{111} + a^2_{222} \right) \] (20)

set the same as \( E_H \) in (5), so we obtain the relation

\[ L^2 = L_{(b)0}^2 \left( 3 - 2^2_{111} + a^2_{222} \right). \] (21)

Substitute (20) to (3) and by using (21), the force in this process is

\[ F^{(B)}_{1x}(L) = F^{(B)}_{1y}(L) = F^{(B)}_{1z}(L) = \frac{3\pi^2 h^2}{mL_{(B)3}^2 L}. \] (22)

Then, the moving-sides of the cubic potential reach the farthest distance when \( L_{(b)2} = 2L_{(b)3} \), in which the particle is excited to the fourth level, \( a_{111} = 0 \) and \( a_{222} = 1 \). Hamiltonian expectation value at the end of this process is given by,

\[ E^{(b)}_2 = \frac{12\pi^2 h^2}{2mL_{(b)2}^4}. \] (23)

The next process is adiabatic expansion which entirely occurs in the third level energy of the system. The force
\[ F_{2s}^{(b)}(L) = F_{2y}^{(b)}(L) = F_{2z}^{(b)}(L) = \frac{12\pi^2\hbar^2}{mL^3} \] (24)

used to push moving-sides up to \( L_{\beta3} = k_{\beta}L_{\beta2} \) with \( k_{\beta} > 1 \). As a consequence of the adiabatic expansion process, the Hamiltonian expectation value decreases to

\[ E_{C}^{(b)} = \frac{12\pi^2\hbar^2}{2mL_{\beta3}^2}. \] (25)

After the adiabatic process, the next process is isothermal compression. In this process, the state change from the fourth level to the ground state. In order to accommodate the Hamiltonian expectation remain constant, so we set (29) equal to (5) and get

\[ L^2 = \frac{L_{\beta3}^2}{4} (3 - 2a_{111}^2 + a_{222}^2). \] (26)

Particle holds the movement of the moving sides with forces

\[ F_{3x}^{(b)}(L) = F_{3y}^{(b)}(L) = F_{3z}^{(b)}(L) = \frac{12\pi^2\hbar^2}{mL_{\beta3}^2 L} \] (27)

until it reaches maximum compression, \( L_{\beta4} = L_{\beta3}/2 \), when the state returns to ground state. The Hamiltonian expectation value is constant at

\[ E_{4}^{(b)} = E_{C}^{(b)} = \frac{3\pi^2\hbar^2}{2mL_{\beta4}^2}. \] (28)

Furthermore, in the next process, the moving-sides return to initial width \( L_{i} \). During this adiabatic process, the system remains in the ground state. As a result of compression, the Hamiltonian expectation value increases to

\[ E = \frac{3\pi^2\hbar^2}{2mL^2}. \] (29)

We obtain the force at the end of the process is

\[ F_{4x}^{(b)}(L) = F_{4y}^{(b)}(L) = F_{4z}^{(b)}(L) = \frac{3\pi^2\hbar^2}{mL^2}. \] (30)

2.3 Quantum Carnot Engine Model C

The model C of heat engine has the highest transition state compare to the model A and B. The state of the system is a linear combination of ground state, third excitation, and fourth excitation, represent in the form

\[ \Psi^{(c)} = a_{111}\psi_{111} + a_{311}\psi_{311} + a_{131}\psi_{131} + a_{113}\psi_{113} + a_{222}\psi_{222} \] (31)

and \( a_{111}^2 + a_{311}^2 + a_{131}^2 + a_{113}^2 + a_{222}^2 = 1 \). The thermodynamic cycle of the model C is same as the two previous models. First, this engine expands isothermally with the Hamiltonian expectation value remains constant, so we set \( E^{C}(L) \)
equal to $E_H$ in (5) in order to obtain the relation

$$L^2 = \frac{L_{(C)}^2}{3} \left( 1 - 8a_{111}^2 + a_{222}^2 \right).$$

(33)

We substitute (32) into (3) and use the relation (33) to get the force

$$F_{1_x}^{(C)}(L) = F_{1_y}^{(C)}(L) = F_{1_z}^{(C)}(L) = \frac{3 \pi^2 \hbar^2}{m L_{(C)}^2 L}. \quad (34)$$

Then, the cubic potential moving-sides expand until achieved $L_{(C)2} = 2L_{(C)1}$, which is in the third state $a_{111} = 0$ and $a_{222} = 0$. Energy at the end of this process is

$$E_2^{(C)} = \frac{12 \pi^2 \hbar^2}{2 m L_{(C)2}^2}. \quad (35)$$

After that, the system continues the thermodynamic process with adiabatic expansion. During adiabatic process, the system occurs in the third state. The Force

$$F_{2_x}^{(C)}(L) = F_{2_y}^{(C)}(L) = F_{2_z}^{(C)}(L) = \frac{12 \pi^2 \hbar^2}{m L^3} \quad (36)$$

use to expand the moving sides until satisfied the condition $L_{(C)3} = k_{(C)}L_{(C)2}$, with $k_{(C)} > 1$. The Hamiltonian expectation value decreases to,

$$E_{C}^{(C)} = \frac{12 \pi^2 \hbar^2}{2 m L_{(C)3}^2}. \quad (37)$$

as adiabatic expansion result. The final process is isothermal compression in which the Hamiltonian expectation value remains constant. In order to satisfy that, we set (37) equal to (35) to get,

$$L^2 = \frac{L_{(C)3}^2}{12} \left( 1 - 8a_{111}^2 + a_{222}^2 \right). \quad (38)$$

The Force

$$F_{3_x}^{(C)}(L) = F_{3_y}^{(C)}(L) = F_{3_z}^{(C)}(L) = \frac{12 \pi^2 \hbar^2}{m L_{(C)3}^2 L} \quad (39)$$

compress the system until reaches $L_{(C)4} = L_{(C)3}/2$, or when the state turns back to the initial state. The Hamiltonian expectation value has not changed, which is equal to

$$E_4^{(C)} = E_C^{(C)} = \frac{3 \pi^2 \hbar^2}{2 m L_{(C)4}^2}. \quad (40)$$

The last process in a single cycle is adiabatic compression. The Force
push the moving sides return to the initial width $L_i$. During this compression, the system remains in the ground state. and the Hamiltonian expectation value increases to

$$E = \frac{3\pi^2\hbar^2}{2mL^2}.$$  

(42)

3. RESULT AND DISCUSSION

The forces of the same quantum thermodynamic process in each model have identical magnitudes. As a consequence, we can calculate the works done by heat engines in general formalism through the relation as follow

$$W^{(i)} = 3 \left[ \int_{L_{(i)i}}^{2L_{(i)i}} F_{1s}^{(i)}(L) dL + \int_{L_{(i)i}}^{L_{(i)i}} F_{2s}^{(i)}(L) dL + \int_{L_{(i)i}}^{L_{(i)i}} F_{3s}^{(i)}(L) dL + \int_{L_{(i)i}}^{L_{(i)i}} F_{4s}^{(i)}(L) dL \right]$$  

(43)

with, $i = A, B, C$ is the index for all three models. So the works are

$$W^{(i)} = \frac{9\pi^2\hbar^2(\ln 2)}{m} \left( \frac{1}{L_{(i)i}^2} - \frac{4}{L_{(i)i}^2} \right).$$  

(44)

From (1) to get the efficiency of a heat engine, we also must calculate the amount of energy absorbed $Q$ into the system, in general for all models we get

$$Q_{Abs}^{(i)} = 3 \left[ \int_{L_{(i)i}}^{2L_{(i)i}} F_{1s}^{(i)}(L) dL \right] = \frac{9\pi^2\hbar^2}{mL_{(i)i}^2} \ln 2$$  

(45)

Furthermore, the efficiencies are written in the form

$$\eta^{(i)} = 1 - 4 \left( \frac{L_{(i)i}}{L_{(i)i}} \right)^2 = 1 - 4\gamma^{(i)}$$  

(46)

by assuming $\left( \frac{L_{(i)i}}{L_{(i)i}} \right)^2 = \gamma^{(i)}$. By substituting the cold energy $E_C$ and hot energy $E_H$ into (46) for each model, we have the efficiency of all heat engine models similar to previous result (Bender et al., 2000); (Belfaqih et al., 2015); (Sutantyo et al., 2015) as represent in (2)

$$\eta^{(i)} = 1 - \frac{E_C}{E_H}.$$  

(47)
width and the final width of the potential well after isothermal expansion process complete (Saputra and Purwanto, 2010). Another quantity reviewed is the gradient of the efficiency, shown in eq. (46). If all models have the same gradient, which is 4; therefore, all models have the same efficiency (Belfaqih et al., 2015); (Sutantyo et al., 2015). Because the working substance obey quantum nature, QHE has unusual and exotic properties. For example, under some conditions, QHEs can surpass the maximum limit on the amount of work done by a classical thermodynamic cycle (Kieu, 2006) and also surpass the efficiency of a classical Carnot Engine cycle.

4. CONCLUSION

We have shown the efficiency of QHE based on Carnot cycle have the same gradient for all three different models. We can conclude that the effect of the degenerate state does not exist explicitly due to the contribution of the transition state reduce by completeness relation. This result can be generalized to any number of transition states applied to the system; in other words, generally applies to the multistate system. However, the effect of degenerate state can easily exist if we consider it in the highest state. Further research and more discussion are needed outside this manuscript. We still work to consider the degree of degeneration in the transition state and highest state.

REFERENCES


