Quantum Lenoir Engine with a Multiple-eigenstates Particle in 1D Potential Box

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Abstract. QLE which has the working substance of a quantum system, a single particle confined in a one-dimensional potential box, has been constructed theoretically in this paper. The quantum system replaces the role of the classical system which has a working substance in the form of gas confined in a piston cylinder. The piston that moves back and forth is substituted by a 1D potential box wall that can move freely to change the width of the potential box. In this way, the three classical thermodynamic processes in the CLE (Classical Lenoir Engine), namely isochoric, isotherm, and isobar, can be analogous to the quantum system. Finally, we find that the thermal efficiency formulation of QLE has a similarity of shape to the CLE efficiency equation. However, a higher ratio of specific heat for QLE makes the efficiency value greater than CLE at each same compression ratio.

Keywords: QLE (Quantum Lenoir Engine), efficiency, potential box, compression ratio, ratio of specific heat

1. Introduction
The heat engine that has been used by the public uses a working substance in the form of an ideal gas in a piston-cylinder. This heat engine can transform the heat entering the system into work with an efficiency of less than 100%. This is in line with the 2nd law of thermodynamics where there is always residual heat released into the surroundings because it is impossible for all heat entering the system to be converted into work by a heat engine [1].

In this era, the working fluid of a heat engine, which is generally a classic system, needs to be replaced to increase the efficiency of the engine. One alternative replacement is a quantum system that works on a microscopic scale. Some quantum systems that have been investigated as substitute working substances for classical systems are potential box [2]–[9], oscillator harmonic [10], quantum dot [11], quantum Rabi model [12], optical cavity [13], etc.

The Lenoir engine was an internal combustion engine that was first commercialized by Étienne Lenoir in 1860. This engine became the forerunner of other commercial heat engines such as the Carnot engine, Otto engine, Brayton engine, Diesel engine, etc. This engine has three thermodynamic states for each cycle, ie isochoric, adiabatic expansion, and isobaric compression [14]. CLE also uses the ideal gas as the working fluid which is in a piston tube.

The replacement of working fluid in QLE will be applied in this research theoretically. The ideal gas in the piston tube will be replaced by a quantum system, a multiple-eigenstates particle that is in the 1D potential box [2]. The replacement requires adjustment of thermodynamic variables in the classical system into the quantum system. Three thermodynamic processes of each cycle in CLE also need to be harmonized in QLE.
This theoretical research, using a quantum system, is research-based on future technology in the field of energy conversion. We hope that it will become one of the cornerstones in the research of quantum systems as a working fluid to outperform the efficiency of heat engines, that previously used a classical system as its working fluid. Besides, it will be in line with current technological developments that increasingly lead to the microscopic realm where quantum systems play a major role in this area.

This paper is arranged as follows: This research begins with the description of the quantum system as a modified analogy of the classical system. Then, the variables that appear in the classical thermodynamic system are analogous to the quantum thermodynamic system. The net work and heat energy absorbed by the quantum system in each QLE cycle are derived analytically. Finally, the formulation efficiency of QLE is obtained and compared with CLE at the same compression ratio. QLE reversibility rate is calculated based on the modified Clausius inequality for this quantum system. The relationships of power per cycle to the compression ratio and QLE efficiency is also investigated.

2. 1D Potential Box as a Pistoned Cylinder

This research is theoretical research based on the study of literature on a quantum system, namely a single particle with a neglected spin that moves in a 1D potential box. Based on figure 1, the behavior of a single particle with mass m is represented by an eigenfunction $\phi(x)$ in the 1D time-independent Schrödinger equation,

$$\frac{d^2 \phi(x)}{dx^2} + \frac{2mE}{\hbar^2} \phi(x) = 0 \quad (1)$$

with $x$ is particle position, $E$ is total energy (Hamiltonian) of the system, and $\hbar$ is Dirac constant. By applying the boundary conditions at both walls of the box potential whose width is $L$, $\phi(x = 0) = 0$ and $\phi(x = L) = 0$, solution of Equation (1) is

$$\phi_n(x) = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin \frac{n\pi x}{L} \quad (2)$$

where $n$ is the quantum number of values 1, 2, 3, ... Each quantum number has the total energy spectrum of the $n$-th, as the expectation value of Hamiltonian for any quantum state,

$$E_n(L) = \langle \phi_n | \hat{H} | \phi_n \rangle = \frac{\pi^2 \hbar^2}{2mL^2} n^2. \quad (3)$$

$E_1$ is the ground state energy, $E_2$ is the first excited state energy, $E_3$ is the second excited state energy, and so on. According to Equation (3), we can see that the energy spectrum $E_n$ is a function of the quantum number and the width of the potential box.
Figure 1. A particle in the 1D box potential as an analogy to an ideal gas in a piston tube

Eigenfunction set superposition Equation (2) form a complete solution of Equation (1) called the wave function of the system,

$$\psi (x) = \sum_n a_n \phi_n (x)$$  \hspace{1cm} (4)

where $a_n$ is the $n$-th complex coefficient of $\phi_n(x)$. Each complex coefficient is constrained by the normalization condition of the wave function Equation (4),

$$\langle \psi | \psi \rangle = \sum_n |a_n|^2 = 1.$$  \hspace{1cm} (5)

The average total energy (hamiltonian) of a single particle, based on Equation (4), is

$$E(L) = \langle \psi | \hat{H} | \psi \rangle = \sum_n |a_n|^2 E_n (L) = \frac{\pi^2 \hbar^2}{2mL^2} \sum_n \left(n^2 |a_n|^2 \right).$$  \hspace{1cm} (6)

We know that $|a_n|^2$ is the probability of finding the particle in the energy state $n$-th. The potential wall mechanical force is a negative value from the first differential Equation (6) with respect to the width of the potential box,

$$F(L) = -\frac{dE(L)}{dL} = \frac{\pi^2 \hbar^2}{mL^2} \sum_n \left(n^2 |a_n|^2 \right).$$  \hspace{1cm} (7)
From Equation (7), we know that the greater the quantum number $n$, the $F(L)$ will be greater as well, while the wider the box potential will decrease the value of $F(L)$. Bender et al. have succeeded in modifying the relationship of the quantities of heat engines in the classical system with its quantum system [15]. The gas pressure is analogous to the driving force of the potential box wall, the volume of the cylinder is analogous to the width of the potential box, and the gas temperature is analogous to the expectation value of the hamiltonian of the quantum system. This makes the graph $P(V)$ can also be analogous to $F(L)$ with the work of each quantum thermodynamic process can be calculated as the area under the graph $F(L)$,

$$W = \int F dL.$$  

(8)

3. Thermodynamics Law of Quantum System

The first law of classical thermodynamics states that the change in the internal energy ($dU$) of an ideal gas is the difference between the heat energy ($dQ$) entering or leaving a system against the work ($dW$) done or imposed on the system,

$$dU = dQ - dW.$$  

(9)

This law can be analogous to this quantum system by treating the expectation value of the total energy of the system, Equation (6), as internal energy. Therefore, the change in total energy can be expressed as

$$dE = \sum_{n} E_n d\left(|a_n|^2\right) + \sum_{n} |a_n|^2 dE_n$$  

(10)

where according to Equation (9), the first term of the right-hand side is heat energy while the second term of the right-hand side is the negative value of work,

$$dQ = \sum_{n} E_n d\left(|a_n|^2\right) \quad \text{and} \quad dW = -\sum_{n} |a_n|^2 dE_n.$$  

(11)

The sign convention: The heat energy entering the system is positive and negative if it leaves the system into the surroundings. Work will be positive if the system does work to the surroundings and vice versa.

4. Quantum Lenoir Engine

As well as the classic heat engine in which each cycle is generally expressed in the graph of $P(V)$, it would be better if QLE is also expressed in graph $F(L)$ so that each process is easy to understand (figure 2). The QLE cycle consists of an isochoric process by the absorption of heat from the
surroundings, an adiabatic process by releasing work into the surroundings, and the isobar compression process by releasing heat into the surroundings.

![Diagram](image)

**Figure 2.** (a) Graph F(L) for each QLE cycle, (b) Eigenstates occupied by a single particle in each quantum thermodynamic process

First, suppose a single particle is in the ground state (n = 1) at point A. The particle will have a wave function $\psi = \phi_1$ with an expectation value of total energy $E = E_1$. In one cycle, a single particle will experience changes in wave function and total energy until finally returning to point A. Every quantum thermodynamic process is considered to take place in a quasistatic and reversible condition so that Equation (2) can still be applied to this system. The thermal efficiency of QLE can be determined after previously $Q_{in}$ and $W_{net}$ can be calculated.

### 4.1. Step AB

A single particle absorbs $Q_{in}$ so that it increases in total energy from the ground state (n = 1) to the superposition states (n = 1, 2, 3, ..., $n_f$) without changing the width of the potential box. The wave function and the expectation value of the total energy of the system, i.e.

$$\psi_{AB}(x) = a_1\phi_1(x) + a_2\phi_2(x) + a_3\phi_3(x) + \cdots + a_{n_f}\phi_{n_f}(x)$$

(12)

and

$$E_{AB}(L) = \sum_{n=1}^{n_f} |a_n|^2 E_n(L) = \frac{\pi^2\hbar^2}{2mL^2} s_f$$

(13)
in which \( s_f = \sum_{n=1}^{n_f} \left( n^2 |a_n|^2 \right) \). Because no work arises during this isochoric process, \( Q_{in} \) is used entirely to raise the internal energy of the quantum system from point A to C,

\[
Q_{in} (L) = \Delta U_{AC} = E_C - E_A = \frac{\pi^2 \hbar^2}{2mL_A^2} (s_f - 1) \tag{14}
\]

which is positive (as a sign that heat enters the system).

4.2. Step BC
Particles undergo a quantum adiabatic process so that the probability of each eigenfunction composing BC does not change during this process, \( |a_n|^2 \) is constant for every possible \( n \) value, even though the width of the potential box is expanded from \( L_B = L_A \) to \( L_C \). The wave function and total energy of the particle during the BC process are

\[
\psi_{BC} (x) = \sum_{n=1}^{n_f} a_n \phi_n (x) \tag{15}
\]

and

\[
E_{BC} (L) = \frac{\pi^2 \hbar^2}{2mL^2} s_f, \tag{16}
\]

The force that widens the potential box, the negative value of the first differential Equation (16) with respect to \( L \), is

\[
F_{BC} (L) = \frac{\pi^2 \hbar^2}{mL^3} s_f. \tag{17}
\]

The work done by the system to the surroundings, which is a positive value, can be obtained

\[
W_{BC} = \int_{L_B=L_A}^{L_C} F_{BC} dL = \frac{\pi^2 \hbar^2}{2m} s_f \left( \frac{1}{L_A^2} - \frac{1}{L_C^2} \right) \tag{18}
\]

4.3. Step CA
The potential box is compressed from \( L_C \) to \( L_A \) so the system releases \( Q_{CA} \) to the surroundings in a condition of constant compression force. A single particle de-excite from a superposition states (\( n = 1 \),
2, 3, ..., \( n \)) back to the ground state (\( n = 1 \)). The wave function and the expectation value of the total energy of the system in this isobar process are, respectively

\[
\psi_{CA}(x) = \sum_{n=1}^{n_f} a_n \phi_n(x) \quad (19)
\]

and

\[
E_{CA}(L) = \frac{\pi^2 \hbar^2}{2mL^2} s_f. \quad (20)
\]

The compression force is always constant during this process, \( F_{CA} = F_A = 0 \), so we find a relation of the width of the potential box during the CA process to the width of the initial box,

\[
L = s_f^{1/3} L_A. \quad (21)
\]

The work done from surroundings to the system is

\[
W_{CA} = \int_{L_c}^{L_A} F_{CA} dL = -\frac{\pi^2 \hbar^2}{mL_A^2} \left( s_f^{1/3} - 1 \right) \quad (22)
\]

which is negative. Change in quantum internal energy can be determined by calculating the energy difference at the beginning and the end of the CA process,

\[
\Delta U_{CA} = E_A - E_C = -\frac{\pi^2 \hbar^2}{2mL_A^2} \left( s_f^{1/3} - 1 \right) \quad (23)
\]

which is negative. Finally, \( Q_{out} \) can be calculated based on Eq (9),

\[
Q_{CA} = \Delta U_{CA} + W_{CA} = -\frac{3\pi^2 \hbar^2}{2mL_A^2} \left( s_f^{1/3} - 1 \right) \quad (24)
\]

which is also a negative value (heat out of the system).

**4.4. Efficiency Calculation**
The total work done for one cycle can be calculated by summing work in all three quantum thermodynamic processes,

\[ W_{net} = \oint F dL = \frac{\pi^2 h^2}{2mL_A^2} [f(\gamma f - 1) - 3(f^{1/3} - f)] \]. \hspace{1cm} (25)

Efficiency is defined as a ratio of Equation (25) to Equation (14),

\[ \eta = 1 - 3\left(\frac{L_C}{L_A}\right)^3 - 1 \]. \hspace{1cm} (26)

with \( \gamma = 3 \) is the ratio of specific heat for this quantum system. Meanwhile, the compression ratio is defined by considering Equation (21) as

\[ r = \frac{L_C}{L_A} = f^{1/3} = \left[ \sum_{n=1}^{n_{\text{in}}} \left( n^2 |a_n|^2 \right) \right]^{1/3} \]. \hspace{1cm} (27)

5. Clausius Relation of QLE
Reversibility behavior of a heat cycle with a classical system has been formulated by Rudolf Clausius (in 1865) and known as Clausius inequality [14],

\[ \oint \frac{dQ}{T} \leq 0 \] \hspace{1cm} (28)

where \( Q \) is the heat energy entering or leaving a classical system and \( T \) is the temperature of its system. A closed integral is zero if the cycle is reversible and less than zero if it is irreversible. Bender et al. has modified Equation (28) for the quantum system which is written as

\[ \oint \frac{dQ}{E} = \frac{Q_{\text{in}}}{E_{\text{hot}}} + \frac{Q_{\text{out}}}{E_{\text{cold}}} \leq 0. \] \hspace{1cm} (29)

Equation (29) is not intended to calculate the value of entropy change during a given heat cycle, but only to describe its reversibility rate.
To calculate the reversibility rate of QLE, we first know that this engine operates on two energy bath, namely the heat energy bath and the cold energy bath,
Equations (14) and (24) give an amount of heat energy entering and leaving the quantum system. We get

\[ E_{\text{hot}} = \frac{\pi^2 \hbar^2}{2mL_A} r^3 \quad \text{and} \quad E_{\text{cold}} = \frac{\pi^2 \hbar^2}{2mL_A}. \quad (30) \]

Equation (31) shows the dependence of the closed integral value (entropy change) on the compression ratio \( r \), plotted in figure 3.

\[ \oint \frac{dQ}{E} = 4 - 3r - \frac{1}{r^3}. \quad (31) \]

6. Power of QLE

The relationship between power and efficiency of the QLE in each cycle can be determined as follows. We initially derive the total change in potential box width, \( \Delta L \), for each QLE cycle,

\[ \Delta L = (L_B - L_A) + (L_C - L_B) + (L_C - L_A) = 2(L_C - L_A). \quad (32) \]

The average speed of a potential box in one cycle is written as

\[ \bar{v} = \frac{\Delta L}{\tau} = \frac{2(L_C - L_A)}{\tau}. \quad (33) \]

where \( \tau \) is the period of the QLE cycle. From Equation (33), the period of the QLE cycle is

\[ \tau = 2(L_C - L_A)/\bar{v}. \]

The power in a QLE cycle is defined as the amount of net work per cycle period,
The relationship of power and compression ratio on Equation (34) can be developed into a relationship of power and efficiency according to Equation (27),

\[ P = \frac{\pi^2 \hbar^2 V}{4mL_A^3} \left( r + 2 \right) \left( r - 1 \right). \]  

Finally, Equations (34) and (35) are illustrated in figure 4.

![Figure 4](attachment:image.png)

**Figure 4.** (a) Graph of power vs compression ratio, (b) Graph of power vs efficiency

### 7. Results and Discussion

The efficiency of QLE for the case of superposition of the eigenstates (n = 1, 2, 3, ..., n), according to Equation (26), has the same form as the efficiency of the CLE version (Table 1) [16]. The difference is in the value of the ratio of specific heat wherein this quantum system is \( \gamma = 3.0 \) while for the diatomic gas system, which is often used in classical engine systems, is \( \gamma = 7/5 \).

### Table 1. QLE efficiency vs CLE efficiency

| General Form | QLE \((\gamma = 3)\) | CLE \((\gamma = 7/5)\) |
|--------------|----------------------|-------------------------|
| \( \eta = 1 - \gamma \frac{r - 1}{r' - 1} \) | \( \frac{L_C}{L_A} - 1 \) | \( \frac{V_C}{V_A} - \frac{1}{5} \) |
| \( \eta = 1 - 3 \left( \frac{L_C}{L_A} \right)^3 - 1 \) | | |
| \( \eta = 1 - \frac{V_C}{V_A} \left( \frac{V_C}{V_A} \right)^{-1} \) | | |
At the same compression ratio, the efficiency graph as a function of the ratio of specific heat is illustrated in figure 5. From this graph, we find that for all four values of the same compression ratio, QLE is always more efficient than CLE. Also, the higher the value of the compression ratio, the higher the value of QLE and CLE efficiency. According to Equation (27), the compression ratio will increase if the particle rises to a higher excited state.

![Efficiency Graph](image)

**Figure 5.** Graph of efficiency vs ratio of specific heat for QLE and CLE

The efficiency of QLE for multiple-eigenstates is equivalent to the equation of QLE efficiency for cases where there are only two eigenstates, namely the initial and final eigenstates [17]. Then, if the potential box is stretched until it reaches its maximum value, the particle will reach a single state (no longer a superposition of eigenstates), i.e. the eigenstate for \( n = n_f \) with \( L_{C,max} = h_f^{2/3} L_A \). This means that multiple-eigenstates QLE can be seen as two eigenstates QLE for this condition. Figure 3 shows that QLE is irreversible because the closed integral value is less than zero for \( r > 1 \). The irreversible rate depends on the compression ratio worked on this engine. The higher the ratio \( L_C \) and \( L_A \), QLE is getting irreversible. Based on Equation (27), when the compression ratio is increased, the particle will reach the highest excited state \( (n_f) \) again.

The power to compression ratio and efficiency relationships have been plotted in Figure 4. It says that the greater the compression ratio applied to QLE will increase the power that can be extracted per cycle. Efficiency enhancement of the QLE also has the effect of increasing engine power.

So far, we have examined the efficiency of the Lenoir engine with the working substance of a quantum system of the particle in a 1D potential box. This Lenoir engine is one of the simplest heat engines because it only consists of three steps while other engines reach four steps (Carnot engine, Otto engine, Brayton engine, Diesel engine, etc.) even up to five steps (dual engine) in each cycle. The simplicity of the steps of this engine will provide a great opportunity to be constructed first compared to other heat engines with the working fluid in the form of a quantum system, a potential box, a quantum harmonic oscillator, a quantum dot, etc. In the future, heat engines with quantum systems are expected to enhance the value of thermal efficiency compared to classical heat engines. This will be in line with current technological developments that have reached the microscopic and even nanoscopic scale.

### 8. Conclusion

The QLE efficiency formulation, both for multiple-state cases and two eigenstate cases is similar to the CLE efficiency formulation. A greater ratio of specific heat for QLE than CLE causes the QLE efficiency value to exceed CLE efficiency if applied to the same compression ratio. Increasing the value of the compression ratio will increase the efficiency of QLE and CLE, but decrease the
reversibility rate of both. Then, if the width of the well can reach its maximum value, multiple-eigenstates QLE can be treated as two eigenstates QLE. Increasing QLE efficiency is also followed by an increase in power per cycle.

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