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The performance analysis of a Wood-Saxon driven Quantum-Mechanical Carnot Engine

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Abstract: *Classical heat engines (CHEs) have long been employed to convert heat energy into mechanical work through various thermodynamic processes. However, limitations such as friction have driven the exploration of quantum heat engines (QHEs), which operate in the quantum domain and are less susceptible to classical constraints. In this study, we focus on Quantum Heat Engines powered by the Wood-Saxon (WS) oscillator, a model originally developed for nuclear physics but recently applied to quantum systems. Building upon previous work on the efficiency of a WS-powered Carnot engine, we further investigate its performance optimization. We derive expressions for the dimensionless power output and explore the optimization of power output and efficiency. Through mathematical analysis, we determine the optimal parameters for maximum power output, considering the condition for non-negativity of efficiency. The dimensionless power output is found to depend on the efficiency, which varies with the characteristics of the working substance. Our results show that the Wood-Saxon model outperforms the Free Particle model in terms of maximum power efficiency for Quantum Carnot engines. The efficiency at maximum power for the WS-powered engine is 0.739, indicating its superiority over the Free Particle model. This analysis provides insights into the performance characteristics of quantum heat engines and underscores the significance of the choice of working substance in optimizing engine efficiency.*

Keywords: *Quantum thermodynamics, Wood-Saxon, Carnot cycle, Quantum heat engines, finite-engine.*

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1.0 Introduction

Classical heat engines CHEs are systems designed to convert heat energy to useful energy particularly mechanical energy which is used to do work W. This conversion is possible with the introduction of a working substance which is subjected to a cyclic process between two reservoirs at different temperatures i.e., from high-temperature T_H to low temperature T_L. However, the arrangement of these processes such as the isochoric, adiabatic, isothermal, isoenergetic etc. for any particular engine leads to several types of cycles which is referred to as engine cycle e.g., the Carnot cycle which consists of isothermal with isentropic (reversible adiabatic) process while Otto and Brayton's cycles are made up of isobaric with adiabatic and isochoric with adiabatic processes respectively.

The limitation of CHE caused by friction and drags has led to the development of quantum versions of heat engines often referred to as Quantum heat Engines QHE. The latter is governed by Quantum fluctuation thereby becoming immune from the former's limitation since the energy exchange between the system and thermal reservoirs at this scale occurs in the quantum domain where the law of classical physics breakdown (Abah *et al.*, 2012; Campisi *et al.*, 2011; E. O. Oladimeji *et al.*, 2023; Peterson *et al.*, 2019; Von Lindenfels *et al.*, 2019). However, to understand the quantization concept of heat engines, we are not free from the classical analogous description of these engines since the quantum regime energy transfer is governed by the second law of thermodynamics (Alicki, 1979; Dann & Kosloff, 2020; Gelbwaser-Klimovsky *et al.*, 2013; Gemmer *et al.*, 2009; Kosloff, 2013; Vinjanampathy & Anders, 2016). This miniaturized heat engine i.e., Quantum Heat Engine QHE as its classical counterpart also consists of basic thermodynamic processes and its physical quantities at a constant temperature, entropy, volume, pressure, and energy which correspond to these processes. But the fuel that drive these QHE are referred to as working substance are mathematical models i.e., Free-Particle (Bender *et al.*, 2000; Guzmán-Vargas *et al.*, 2002), Harmonic Oscillators (Deffner, 2018; Deffner & Lutz, 2008; Fei *et al.*, 2022; Kosloff & Rezek, 2017), Pöschl-Teller Oscillator (E. Oladimeji *et al.*, 2021; E. O. Oladimeji, 2019), Morse Oscillator (E. O. Oladimeji, Idundun, *et al.*, 2024), Wood-Saxon (E. O. Oladimeji, Ibrahim, *et al.*, 2024) (our working substance of interest) etc.

The Wood-Saxon WS oscillator was introduced in 1954 by *Wood* and *Saxon* study nuclear structure and reaction properties (Woods & Saxon, 1954). However, it has proved of recent to be a useful model for analysing nonlinearities in quantum systems (Aytekin *et al.*, 2013; Horchani *et al.*, 2022), which became evident by its application in Quantum engine systems by *Oladimeji et al.*(E. O. Oladimeji, Ibrahim, *et al.*, 2024). In their work, they made an intriguing discussion about a quantum-mechanical analogue of the Carnot cycle using WS as a working substance for a Carnot cycle where they constructed an adiabatic and isothermal quantum analogous process and reduced their derived result to well-known potential i.e., Free-Particle FP.

Following the derivation of their efficiency of a Carnot Heat engine using the WS as a working substance by *Oladimeji et al* (E. O. Oladimeji, Ibrahim, *et al.*, 2024), we improved their result as we observed the problem of optimizing the power output P, the possible optimum power P_m^* and its efficiency η_m^* of the same engine is derived. To achieve this, the engine shall become a finite system when time τ of a cycle is introduced.

This work is arranged as follows: in section II, we calculate our engine's dimensionless power output (p^*); in section III, we xamine the optimal power value oncerning engine's efficiency; and in section IV, we draw our conclusions.

2.0 The Carnot cycle

The Carnot cycle (Fig. 1) is an excellent representation of a reversible heat engine and is generally acknowledged as the most efficient cycle achievable under physical law, though it is virtually hard to implement in real engines.

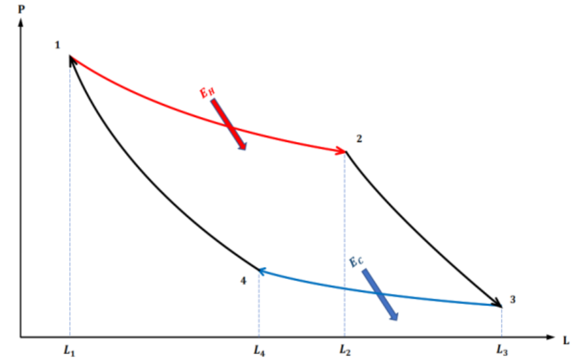

Fig. 1: The schematic representation of a quantum heat engine cycle in the plane of the width (L) and Pressure P(L). The cycle consists of two (2) isoenergetic and two (2) adiabatic processes.

The cycle is composed of two types of thermodynamic reversible processes namely, isothermal and adiabatic processes. The cycle stays in equilibrium throughout an isothermal process i.e., both the temperature T and the internal energy U of the gas remain constant, and work is done as the system remains in contact with the heat source as the gas expands. While during the adiabatic process, the system is isothermally isolated and remains in equilibrium as some of its internal energy U of the gas is converter useful work W.

The work is extractable and the efficiency η is defined as $\eta = 1 - \frac{E_L}{E_H}$ with $E_H(E_L)$ representing the expectation value of the system Hamiltonian along the analogue of the isothermal process at high (low) temperature.

The Total Work-done W efficiency η_{WS} of the WS-powered Carnot engine is shown to be.

$$W = \left(\frac{{V_o}^2 m L_1^2}{72\hbar^2} - \frac{\hbar^2 \ln\left(\frac{3}{2}\right)}{m{L_1}^2}\right) - \left(\frac{{V_o}^2 m L_3^2}{72\hbar^2} - \frac{9\hbar^2 \ln\left(\frac{3}{2}\right)}{4m{L_3}^2}\right) \quad (1)$$

and

$$\eta_{WS} = 1 - \left(\frac{9L_1^2}{4L_3^2}\right)\left(\frac{\alpha - 1}{\beta - 1}\right) \quad (2)$$

where:

$$\alpha = \frac{4{V_o}^2 m^2 L_3^4}{9\left(72\hbar^4 \ln\left(\frac{3}{2}\right)\right)} \quad \text{and} \quad \beta = \frac{{V_o}^2 m^2 L_1^4}{72\hbar^4 \ln\left(\frac{3}{2}\right)}$$

The Wood-Saxon's efficiency η_{WS} reduces to that of Free Particle η_{FP} by setting the potential depth $V_0 = 0$ (Bender *et al*., 2000; E. Oladimeji *et al*., 2021; E. O. Oladimeji, Ibrahim, *et al*., 2024).

$$\eta_{FP} = 1 - \left(\frac{9L_1^2}{4L_3^2}\right)$$

2.1 Optimization of the performance of the heat engine

The work done W, efficiency η and power output P are the important parameters often considered in the optimal design and theoretical analysis of heat engines (J. Wang, He, & Mao, 2007; J. Wang, He, & Xin, 2007). The total work done by the system and total movement L_{total} per cycle of the heat engine, which is the sum of the work on each process $W = \oint dW = -(W_{AB} + W_{BC} + W_{CD} + W_{DA})$ and $L_{total} = (L_1 - L_2) + (L_2 - L_3) + (L_3 - L_4) + (L_4 - L_1) = L_0$. Therefore:

$$L_0 = 2(L_3 - L_1) \equiv \int_0^\tau dt\, v(t) = \bar{v}\tau \quad (3)$$

where $v(t)$, $\bar{v}$ and τ are the speed, the average speed of the change of L and the total time to complete a cycle τ (Abe, 2011; Peña *et al.*, 2016). However, to avoid defiling the adiabatic theorem, the timescale of the state's variation is taken to be larger than that of the dynamic one $\sim\hbar/E$ (Abe, 2011; E. O. Oladimeji *et al.*, 2023; Peña *et al.*, 2016; J. Wang & He, 2012; R. Wang *et al.*, 2012). Thus, the total cycle time τ is expressed as:$\tau = \frac{L_0}{\bar{v}} = \frac{2}{\bar{v}}(L_3 - L_1)$. Therefore, the power output per cycle is:

$$P = \frac{W}{\tau} = \left\{\left(\frac{V_0^2 m L_1^2}{72\hbar} - \frac{\hbar^2 ln1.5}{mL_1^2}\right) - \left(\frac{V_0^2 m L_3^2}{72\hbar} - \frac{9\hbar^2 ln1.5}{4mL_3^2}\right)\right\} \times \frac{\bar{v}}{2(L_3 - l_1)} \quad (4)$$

Given that, $\alpha = \frac{V_0^2 m\bar{v}}{144\hbar}$ and $\beta = \frac{\hbar^2 \bar{v} ln1.5}{8m}$, therefore:

$$P = \alpha\left(\frac{L_1^2 - L_3^2}{L_3 - L_1}\right) + \beta\left(\frac{9L_1^2 - 4L_3^2}{L_1^2 L_3^3 - L_1^3 L_3^2}\right) \quad (5)$$

$$P = \beta\left(\frac{9L_1^2 - 4L_3^2}{L_1^2 L_3^3 - L_1^3 L_3^2}\right) - \alpha\left(\frac{L_1^2 - L_3^2}{L_3 - L_1}\right)$$

Next, we factor L_1^3 from the denominator of the coefficient of β and using the difference of two squares for the numerator of the coefficients of α, we have.

$$P = \frac{\beta}{L_1^3}\left(\frac{9L_1^2 - 4L_3^2}{\frac{L_3^3}{L_1} - L_3^2}\right) - \alpha\left(\frac{(L_3 - L_1)(L_3 + L_1)}{L_3 - L_1}\right) = \frac{\beta}{L_1^3}\left(\frac{9L_1^2 - 4L_3^2}{\frac{L_3^3}{L_1} - L_3^2}\right) - \alpha(L_3 + L_1) \quad (6)$$

Dividing through the coefficients of β by L_1^2 and coefficients of α by L_1, we have that.

$$P = \frac{\beta}{L_1^3}\left(\frac{\frac{9L_1^2}{L_1^2} - \frac{4L_3^2}{L_1^2}}{\frac{L_3^3}{L_1^3} - \frac{L_3^2}{L_1^2}}\right) - \alpha L_1\left(\frac{L_3}{L_1} + \frac{L_1}{L_1}\right) \quad (7)$$

Given that $r = L_3/L_1$, where L_1 and L_3 are assumed to be fixed and variable parameters respectively, thus the power output of the engine P is:

$$P = \frac{\beta}{L_1^3}\left(\frac{(3 - 2r)^2}{r^3 - r^2}\right) - \alpha L_1(r + 1) \quad (8)$$

To derive the maximum power in equ. (8), we set L_1 and $\bar{v}$ to be fixed given the condition:

$$r = \frac{L_3}{L_1} \geq 2 \quad (9)$$

is satisfied in order for the efficiency to be non-negative (Abe, 2011).

To obtain the dimensionless power P^*, we set the dimensions of the power output to unity.

$$P^* = \frac{W}{s\tau} \quad (10)$$

where s is a constant for the model which has units of power (Peña *et al.*, 2016).

$$P^* = \frac{ln1.5}{8}\left(\frac{9 - 4r^2}{r^3 - r^2}\right) - \frac{1}{144}(r + 1) \quad (11)$$

This also implies that the dimensionless r^* is:

$$r^* = \frac{r}{s} \equiv r_{FP} \quad (12)$$

where r_{FP} is the ratio between L_3 and L_1 for an FP-powered Carnot engine (Abe, 2011; Bender *et al.*, 2000; E. O. Oladimeji, Ibrahim, *et al.*, 2024).

To get the maximum dimensionless power output P_m^*, we need to find the value of P at the point $r = r_{mp}$ which corresponds to the maximization condition $\frac{\partial P^*}{\partial r}\Big|_{r=r_m} = 0$. This condition gives rise to the quintic equation:

$$r^5 - 2r^4 - (72ln1.5 - 1)r^3 + (486ln1.5)r + 324ln1.5 = 0 \qquad (13)$$

which has three real solutions $r_{m_1} = -0.715$, $r_{m_2} = 5.747$ and $r_{m_3} = 3.110$. However, considering the condition in eq. (9), two of the solutions r_{m_2} and r_{m_3} seems to meet the condition with r_{m_2} leading to a higher efficiency η_m^* at maximum power.

$$\eta^* = 1 - \frac{3}{2(5.747)} \cong 0.739 \qquad (14)$$

Inserting the value of r^* into the dimensionless power output P^* as a function of the efficiency, η becomes:

$$P^* = \frac{\ln(1.5)}{8}\left(\frac{2\eta(1-\eta)^{\frac{1}{2}}}{2(1-\eta)^{\frac{1}{2}} - 3}\right) - \frac{1}{144}\left(\frac{3 + 2(1-\eta)^{\frac{1}{2}}}{2(1-\eta)^{\frac{1}{2}}}\right) \qquad (15)$$

It is straightforward to validate the result of the derived energy efficiency of any engine's working substance because they are universal, however, it turns out that derived efficiency η^* at maximum power of all Quantum systems are not similar, that is the value of any model can't be reduced to another model's result because its values depend on the form of the working substance i.e. potential (Abe, 2011; He *et al*., 2012; E. O. Oladimeji, Ibrahim, *et al*., 2024; H. Wang *et al*., 2009; J. Wang *et al*., 2011; J. Wang, He, & Xin, 2007).

In this work, the maximum power efficiency $\eta^*$of our WS-powered Quantum Carnot engine is 0.739 making the WS a better fuel to power our system when compared with its family potential, the Particle-in-a-box model i.e., the Free-Particle FP whose $\eta^* = 0.573977952$ (Abe, 2011). However, the FP-powered quantum Carnot system may still be a favourite for some quantum engine researchers due to its smaller size at $r = 4\cos\frac{2\pi}{9}$.

3.0 Conclusion

This work investigates the performance optimization of a Quantum Heat Engine (QHE) using the Wood-Saxon (WS) oscillator as the working substance, focusing on its power output and efficiency. The study begins with an introduction to classical heat engines (CHEs) and their limitations, leading to the development of QHEs, which operate in the quantum domain. The WS oscillator, initially proposed for nuclear physics, is applied to quantum systems, showing promise in enhancing engine performance.The research derives expressions for the dimensionless power output and explores the optimization of power output and efficiency. Through mathematical analysis, optimal parameters for maximum power output are determined, considering the condition for non-negativity of efficiency. The study reveals the dependence of power output on efficiency, highlighting the importance of the working substance in quantum engine performance.

In conclusion, this study provides valuable insights into the optimization of Quantum Heat Engines powered by the Wood-Saxon oscillator. The derived expressions for power output and efficiency optimization offer a deeper understanding of the performance characteristics of such engines. The analysis demonstrates that the Wood-Saxon model outperforms the Free Particle model in terms of maximum power efficiency for Quantum Carnot engines, with an efficiency of 0.739 at maximum power. The findings indicate that the choice of working substance significantly affects the performance of quantum engines. The Wood-Saxon oscillator emerges as a promising candidate for enhancing engine efficiency. However, further experimental validation and exploration of practical implementations are necessary to fully harness its potential.

In view of the above findings and conclusion, the following recommendations are proposed

(i) Experimental setups implementing the Wood-Saxon oscillator as a working substance should be designed and tested to confirm the predicted performance enhancements.

(ii) **Exploration of Other Potentials** *to in*nvestigate other potential models besides the Wood-Saxon oscillator to expand the understanding of quantum heat engine performance.

(iii) *Exploration of* potential practical applications of Quantum Heat Engines powered by the Wood-Saxon oscillator. Investigate real-world scenarios where such engines could be implemented to improve energy conversion efficiency or power generation in quantum systems.

(iv) Conduction of further theoretical analysis to explore the behavior of Quantum Heat Engines under different conditions and with various working substances. Optimization

(v) *Development of* optimization strategies for quantum engine designs based on the insights gained from this study. This could involve exploring ways to improve efficiency beyond the Carnot cycle or optimizing performance for specific operating conditions.

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Compliance with Ethical Standards Declarations

The authors declare that they have no conflict of interest.

Data availability

All data used in this study will be readily available to the public

Availability of data and materials

The publisher has the right to make the data public.

Competing interests

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Authors' contributions

Oladimeji Enock, Umeh Emmanuel and Idundun Victory developed the conceptualization. Koffa Durojaiye and Obaje Vivian resolved the equations. Petinrin Moses and Adeleke Joshua did the proof reading in addition to interpreting the solution.