

The Efficiency of Quantum-Mechanical Carnot Engine using the Woods-Saxon Model

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Abstract

The quantum engine cycle serves as an analogous representation of classical heat engines for microscopic systems and the quantum regime of thermal devices is composed of a single element. In this work, we examined the Quantum-Mechanical properties of a non-linear quantum oscillator using the Woods-Saxon WS potential, as a working substance of the Carnot cycle. The Quantum-Mechanical analogue of the cycle was constructed using changes in both the width L and the quantum state n of the potential well. Furthermore, the efficiency of the quantum engine, consisting of adiabatic and isothermal processes is derived. Our result shows to be analogous to that of the classical engine and found to agree, within an appropriate limit, with existing results obtained from Free Particle FP Model. Thus, indicating that the WS model can be used as an alternative working substance in Quantum engines.

Keywords: *Quantum thermodynamics, Woods-Saxon, Carnot cycle, Quantum heat engines, Nano-engines.*

1. Introduction

The study of the relation between heat engines and quantum systems as a working mechanism, which is often referred to as Quantum Heat Engines (QHEs) has always been of keen interest (Chen et al., 2020; Feldmann & Kosloff, 2000, 2004; Friedenberger & Lutz, 2017; Geva & Kosloff, 1996; Hardal & Müstecapliolu, 2015; Insinga et al., 2016; Kosloff, 1984; Levy et al., 2020; Quan et al., 2007a; Roßnagel et al., 2016; Whalen et al., 2003) since the concept was introduced in 1959 by *Scovil and Schultz-Dubois* (Scovil & Schulz-DuBois, 1959). Generally, heat engines are known to convert heat energy Q_H to useful work W and its performance quantifiers are the efficiency η and the power output P (Abah & Lutz, 2017). Practically, however, there is a delicate balance between these quantities such that their peaks are not attainable due to heat leaks and/or loss of energy through friction (del Campo et al., 2018; Kosloff & Feldmann, 2002), which in turn devalues the efficiency η of the engine such that $\eta \leq \eta_c$ (Latifah & Purwanto, 2011), where the Carnot efficiency $\eta_c = 1 - T_C/T_H$ given that T_C is the (cold)low temperature in the heat reservoir and T_H the high temperature in the heat reservoir. However, these concerns become insignificant with the QHEs, since its dynamical equations of motion obey the laws of quantum mechanics (Kosloff & Rezek, 2017).

Over fifty years of extensive theoretical studies of the miniaturization of heat engine from macroscale to nanoscale has shown that the limitations of classical heat engines become negligible as its quantum properties become dominant at the latter scale (Abah et al., 2012; Singh, 2020). These studies have employed appropriate quantum equations of motion together with different working substances such as the spin systems (Geva & Kosloff, 1998; Yin et al., 2017), two-level or multilevel systems (Bender et al., 2000; Quan et al., 2007b), particle in a box FP (Bender et al., 2000; Guzmán-Vargas et al., 2002), cavity quantum electrodynamics systems (Quan et al., 2006;

Scully, 2002), coupled two-level systems (Henrich et al., 2007), Harmonic oscillators HO (Abe, 2013; Kosloff & Rezek, 2017), Pöschl-Teller Oscillator PTO (E. Oladimeji et al., 2021; E. O. Oladimeji, 2019; Rudoy & Oladimeji, 2017a), Shortcut-to-Adiabaticity (Abah, 2017; Abah & Paternostro, 2019; Diao et al., 2018) etc. The spin-offs of these earlier works are the fabrication of classical micro heat engines using optomechanical (Hugel et al., 2002), micro-electromechanical (Steeneken et al., 2011; Whalen et al., 2003), and colloidal systems (Blickle & Bechinger, 2012; Roßnagel et al., 2016), however, to date no quantum heat engine has been constructed.

In 2000, *Bender et al.* proposed a quantum mechanical model of a cyclic engine based a single particle confined in an infinite one-dimensional potential well of width L , the temperature T of the engine is replaced by the expectation value of the Hamiltonian E , that is, the ensemble average of the energies of the quantum particle and the walls of the containing potential play the role of the piston in a cylinder containing an ideal gas and the quantum mechanical equivalents of isothermal and adiabatic processes were constructed (Bender et al., 2000). Their concept was used by (Guzmán-Vargas et al., 2002) and in other works where they formulated and applied the Pöschl-Teller PT potential in Carnot (E. Oladimeji et al., 2021), Joule-Brayton and Otto cycles (E. O. Oladimeji, 2019), rather than the FP model used by *Bender et al.*

Following their formulation, we introduce the Woods-Saxon WS model to construct an adiabatic and isothermal quantum analogous process and analyze the efficiency of an idealized reversible heat engine. This potential was introduced in 1954 by Wood and Saxon for studying nuclear structure and reaction properties, however its application in Quantum systems until recently has not been studied extensively (Woods & Saxon, 1954). Its application in simulating confinement of Quantum Dots QDs was first proposed by Costa et al., (1999), where they proved the WS model to be a viable alternative for studying confined quantum systems. *Xie* presented theoretical analysis of an exciton and studied two electrons confined in a quantum dot with the Woods-Saxon potential in (Xie, 2009a) and (Xie, 2009b) respectively. *Lu et al.* examined the effect of an intense, high-frequency laser field on the optical absorption coefficients and the refractive index change for shallow donor impurities in a QD using the WS potential (Lu et al., 2011). *Aytekin et al.* proved that the WS potential gives good description of the properties of Nano-systems since it can be used to model the confinement in quantum systems with considerable success (Aytekin et al., 2013; Horchani et al., 2022). Hence, the WS model has been shown to be suitable for studying nonlinearities in quantum systems and would be of good interest to understand the performance of QHE whose working substance is constrained within this more realistic potential model.

The one-dimensional form of the potential is:
$$V(x) = \frac{-V_0}{1+e^{\frac{(x-L)}{a}}}$$

where V_0 is the depth, L is taken to stand for the confinement width and a is the diffuseness of the interaction. The corresponding quantized energy spectrum takes the form (Berkdemir et al., 2005):

$$E_n(L) = - \left[\frac{V_0}{2} + \frac{(n+1)^2 \hbar^2}{8mL^2} + \frac{V_0^2 mL^2}{2\hbar^2(n+1)^2} \right], \tag{1}$$

where m is the mass of the particle or the working substance.

This paper is organized as follows: In section 2, a model of a quantum Carnot engine consisting of two adiabatic and two isothermal processes using WS potential as the working medium is established while in section 3, the work-done W by the engine its efficiency η is derived. In section 4, we discussed and validated our results by reducing the derived efficiency to that of the Free particle FP, compared our derived result with another known model and presented our conclusion in section 5.

1. The Carnot Cycle

The Carnot cycle is an ideal model of a reversible heat engine with maximum possible efficiency. It is widely accepted as the most efficient cycle attainable by physical law. The cycle is composed of two 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 of the gas remain constant, and work is done as the system remains in contact with the heat source while the gas expands. In the quantum mechanical representations, the initial state $\psi(x)$ is assumed to be a linear combination of eigenstates $\phi_n(x)$, the expectation value of the Hamiltonian remains constant while the size of the potential well changes with the wall's movement. Thus, the expansion coefficient a_n changes such that $E(L)$ remains fixed as L changes:

$$E(L) = \sum_{n=1}^{\infty} |a_n|^2 E_n, \tag{2}$$

where E_n is the energy spectrum and the coefficients a_n satisfies the normalization condition $\sum_{n=1}^{\infty} |a_n|^2 = 1$. The pressure P exerted on this wall as defined by Hellman and Feynman as (Feynman, 1939; Rudoy & Oladimeji, 2017b):

$$\hat{P}_n(L) = -\frac{\partial \hat{E}_n}{\partial L}, \tag{3}$$

where \hat{E} is defined as the energy operator such that the formal relation between pressure \hat{P} and Hamiltonian is $\hat{P}(\hat{x}, \hat{p}, L) = -(\partial/\partial L)\hat{H}(\hat{x}, \hat{p}, L)$.

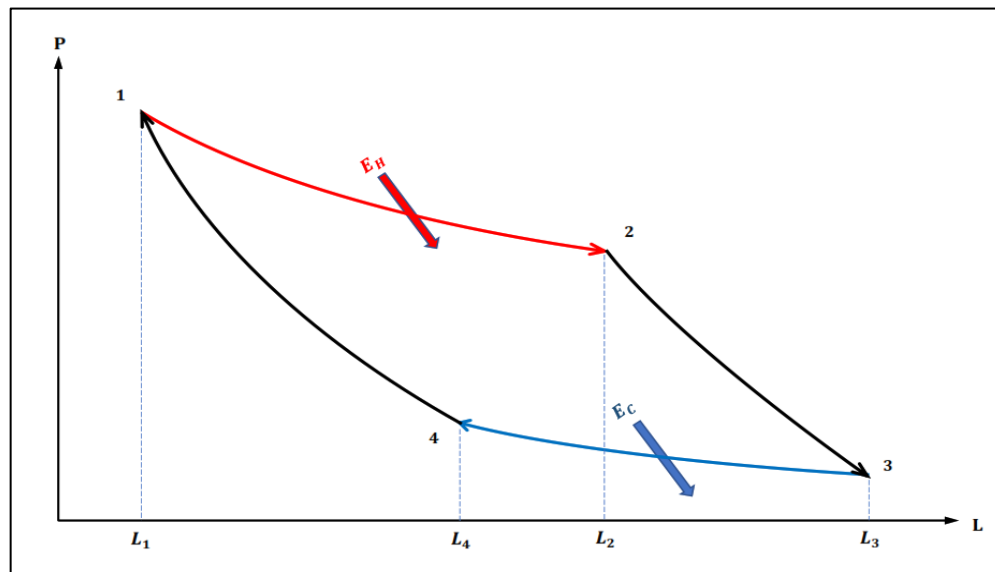


Figure 1: The schematic representation of Carnot's cycle, drawn in (P, L) coordinates (Source: Oladimeji et al., 2021).

1.1 Process 1: Isothermal Expansion

In the first process, the piston is set into an isothermal expansion as the system is excited from its initial state $n = 1$ to the second state $n = 2$ (i.e., from $L = L_1$ to $L = L_2$). This process keeps the expectation value of the Hamiltonian constant and as a result, the state of the system is a linear combination of its two energy eigenstates:

$$\psi_n = a_1(L)\phi_1(x) + a_2(L)\phi_2(x). \tag{4}$$

where ϕ_1 and ϕ_2 are the wavefunctions of the first and second states, respectively. The expectation value of the Hamiltonian is calculated using $E = \langle \psi | H | \psi \rangle$:

$$E(L) = \sum_{n=1}^2 (|a_n|^2)E_n = |a_1|^2E_1 + |a_2|^2E_2. \tag{5}$$

where the coefficients are constrained by the normalization condition $|a_1|^2 + |a_2|^2 = 1$ and E_n ($n = 1, 2, 3, \dots$) maybe obtained from the WS energy spectrum. At $n = 1$ we have that the heat input E_H into the system is

$$E_H = -\left(\frac{V_0}{2} + \frac{\hbar^2}{2mL_1^2} + \frac{V_0^2 mL_1^2}{8\hbar^2}\right). \tag{6}$$

Considering the transition from $n = 1$ to $n = 2$

$$E(L) = \left(\frac{5\hbar^2}{8mL^2} - \frac{5V_0^2 mL^2}{72\hbar^2}\right)|a_1|^2 - \left(\frac{V_0}{2} + \frac{9\hbar^2}{8mL^2} + \frac{V_0^2 mL^2}{18\hbar^2}\right). \tag{7}$$

Since the expectation value is constant during the process, we set the expectation value to be equal to E_H

$$-\left(\frac{V_0}{2} + \frac{\hbar^2}{2mL_1^2} + \frac{V_0^2 mL_1^2}{8\hbar^2}\right) = -\frac{V_0}{2} + \frac{\hbar^2}{8mL^2}[5|a_1|^2 - 9] - \frac{V_0^2 mL^2}{72\hbar^2}[5|a_1|^2 + 4]. \tag{8}$$

Comparing coefficients and solving for L we obtained:

$$L^2 = -\frac{L_1^2}{4}[5|a_1|^2 - 9].$$

$$L^2 = \frac{9L_1^2}{[5|a_1|^2 + 4]}. \tag{9}$$

The maximum value of L is obtained when $L = L_2$. This is at the end of the isothermal expansion process where $|a_1|^2 = 0$. Therefore, from eq. (9)

$$L_2^2 = \frac{9L_1^2}{4} \Rightarrow L_2 = \frac{3}{2}L_1. \tag{10}$$

The pressure during the isothermal expansion is:

$$P(L) = \sum_{n=1}^{\infty} |a_n|^2 P_n = |a_1|^2 P_1 + |a_2|^2 P_2. \tag{11}$$

The pressure undergoes a change of state from $n = 1$ to $n = 2$ as such resulting in:

$$P(L) = \frac{V_0^2 mL}{36\hbar^2} [5|a_1|^2 + 4] + \frac{\hbar^2}{4mL^3} [5|a_1|^2 - 9]. \tag{12}$$

$$P(L) = \frac{V_0^2 mL}{9\hbar^2} - \frac{9\hbar^2}{4mL^3}. \tag{13}$$

Substituting the value of (10) into (12) gives

$$P_1(L) = \frac{V_0^2 mL}{9\hbar^2} - \frac{\hbar^2}{mL_1^2 \cdot L}. \tag{14}$$

The product $LP_1(L) = \text{constant}$. This is an exact quantum analogue of a classical *equation of state*.

1.2 Process 2: Adiabatic Expansion

Next, the system then undergoes an adiabatic expansion from $L = L_2$ until $L = L_3$. During the process, the system maintains the second state at $n = 2$ as no external energy comes into the system. The expectation value of the Hamiltonian is:

$$E(L) = -\left(\frac{V_0}{2} + \frac{9\hbar^2}{8mL_2^2} + \frac{V_0^2 mL_2^2}{18\hbar^2}\right) = E_C. \tag{15}$$

The pressure P as a function of L is:

$$P_2 = \frac{V_0^2 mL}{9\hbar^2} - \frac{9\hbar^2}{4mL^3}. \tag{16}$$

The product $L^3 P_2(L)$ in (16) is a constant and it is considered the quantum analogue of the classical *adiabatic process*.

1.3 Process 3: Isothermal Compression

This process appears to be a reversal of process 1, the system is compressed isothermally from its current (second) state $n = 2$ at point 3 back to its initial state $n = 1$ in point 4 (i.e., from $L = L_3$ until $L = L_4$) while the expectation value of the Hamiltonian remains constant. Thus, the state of the system is a linear combination of its two energy eigenstates.

$$\Psi_n = b_1(L)\phi_1(x) + b_2(L)\phi_2(x),$$

where ϕ_1 and ϕ_2 are the wave functions of the first and second states respectively

$$E(L) = \sum_{n=1}^{\infty} (|b_1|^2 + |b_2|^2)E_n = |b_1|^2 E_1 + |b_2|^2 E_2. \tag{17}$$

The coefficients are constrained by the normalization condition $|b_1|^2 + |b_2|^2 = 1$. The expectation value of the Hamiltonian in this state as a function of L is calculated using $E = \langle \psi | H | \psi \rangle$, which results in:

$$E(L) = -\frac{V_0}{2} - \frac{\hbar^2}{8mL^2} [4 - 5|b_2|^2] + \frac{V_0^2 mL^2}{72\hbar^2} [5|b_2|^2 - 9]. \tag{18}$$

Setting the expectation value to be equal to E_C

$$E_C = -\left(\frac{V_0}{2} + \frac{9\hbar^2}{8mL_3^2} + \frac{V_0^2 mL_3^2}{18\hbar^2}\right), \quad (19)$$

Since the expectation value is constant during the process, set the expectation value is set to be equal to E_L i.e., $n = 2$

$$-\left(\frac{V_0}{2} + \frac{9\hbar^2}{8mL_3^2} + \frac{V_0^2 mL_3^2}{18\hbar^2}\right) = -\frac{V_0}{2} - \frac{\hbar^2}{8mL^2} [4 - 5|b_2|^2] + \frac{V_0^2 mL^2}{72\hbar^2} [5|b_2|^2 - 9], \quad (20)$$

Comparing coefficients and solving for L we obtain:

$$\begin{aligned} L^2 &= -\frac{L_3^2}{9} [4 - 5|b_2|^2], \\ L^2 &= \frac{4L_3^2}{[5|b_2|^2 - 9]}, \end{aligned} \quad (21)$$

The max value of L is obtained when $L = L_4$ and this is achieved in the isothermal compression when $|b_2|^2 = 0$. Therefore, from eq. (21)

$$L_4^2 = \frac{4L_3^2}{9} \equiv L_4 = \frac{2}{3}L_3, \quad (22)$$

The pressure during the isothermal compression is:

$$P_3(L) = \frac{V_0^2 mL}{4\hbar^2} - \frac{9\hbar^2}{4mL_3^2 \cdot L}, \quad (23)$$

The product $LP_3(L) = \text{constant}$. This is an exact quantum analogue of a classical *equation of state*.

1.4 Process 4: Adiabatic Compression

The system remains in its initial state $n = 1$ at point 4 as it undergoes an adiabatic compression process (i.e., from $L = L_4$ until $L = L_1$). The expectation value of the Hamiltonian is then given by:

$$E(L) = -\left(\frac{V_0}{2} + \frac{\hbar^2}{2mL^2} + \frac{V_0^2 mL^2}{8\hbar^2}\right), \quad (24)$$

and the pressure P as a function of L during this process is given as:

$$P_4(L) = \frac{V_0^2 mL}{4\hbar^2} - \frac{\hbar^2}{mL^3}. \quad (25)$$

The product $L^3 P_4(L)$ in (25) is a constant and it is considered the quantum analogue of the classical *adiabatic process*.

2. Work-Done in One Closed Cycle

During one closed cycle, the new work done W by the quantum heat engine is described by the area of the closed loops gotten from the processes i.e., a summation of the individual work done by each process as shown in eqs (14), (16), (23) and (25).

$$W = W_{12} + W_{23} + W_{34} + W_{41}, \tag{26}$$

$$W = \int_{L_1}^{L_2} P_1(L) dL + \int_{L_2}^{L_3} P_2(L) dL + \int_{L_3}^{L_4} P_3(L) dL + \int_{L_4}^{L_1} P_4(L) dL. \tag{27}$$

Recall that: $L_2 = \left(\frac{3}{2}\right)L_1$ and $L_4 = \left(\frac{2}{3}\right)L_3$, therefore:

$$\begin{aligned} W &= \int_{L_1}^{\frac{3}{2}L_1} \left(\frac{V_o^2 mL}{9\hbar^2} - \frac{\hbar^2}{mL_1^2 \cdot L} \right) dL + \int_{\frac{3}{2}L_1}^{L_3} \left(\frac{V_o^2 mL}{9\hbar^2} - \frac{9\hbar^2}{4mL^3} \right) dL, \\ &+ \int_{L_3}^{\frac{2}{3}L_3} \left(\frac{V_o^2 mL}{4\hbar^2} - \frac{9\hbar^2}{4mL_3^2 \cdot L} \right) dL + \int_{\frac{2}{3}L_3}^{L_1} \left(\frac{V_o^2 mL}{4\hbar^2} - \frac{\hbar^2}{mL^3} \right) dL, \end{aligned} \tag{28}$$

$$W = \left(\frac{V_o^2 mL_1^2}{72\hbar^2} - \frac{\hbar^2 \ln\left(\frac{3}{2}\right)}{mL_1^2} \right) - \left(\frac{V_o^2 mL_3^2}{72\hbar^2} - \frac{9\hbar^2 \ln\left(\frac{3}{2}\right)}{4mL_3^2} \right). \tag{29}$$

The efficiency η of a heat engine is defined as.

$$\eta = \frac{W}{Q_H} \tag{30}$$

given that Q_H is the quantity of heat in the hot reservoir and W is the work performed by the classical heat engine which is analogous to the energy absorbed by the quantum engine during the isothermal expansion:

$$Q_H = \int_{L_1}^{L_2} P_1(L) dL, \tag{31}$$

$$Q_H = \left(\frac{V_o^2 mL_1^2}{72\hbar^2} - \frac{\hbar^2 \ln\left(\frac{3}{2}\right)}{mL_1^2} \right). \tag{32}$$

Therefore, the efficiency η of a quantum heat engine obtained by considering a two-state system in a WS potential model is given by;

$$\eta = 1 - \frac{\left(\frac{V_o^2 mL_3^2}{72\hbar^2} - \frac{9\hbar^2 \ln\left(\frac{3}{2}\right)}{4mL_3^2} \right)}{\left(\frac{V_o^2 mL_1^2}{72\hbar^2} - \frac{\hbar^2 \ln\left(\frac{3}{2}\right)}{mL_1^2} \right)}, \tag{33}$$

which may be rewritten as

$$\eta = 1 - \left(\frac{9L_1^2}{4L_3^2} \right) \left(\frac{\alpha - 1}{\beta - 1} \right), \tag{34}$$

where:

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

Eq. (34) shows that the efficiency obtained with the more realistic WS model takes the same form as in the case of the harmonic oscillator and the free particle models (Abe, 2013; Bender et al., 2000; E. Oladimeji et al., 2021) albeit with a richer insight depending on the magnitude of the factor $9(\alpha - 1)/4(\beta - 1)$.

3. Results and Discussion

It is well known that the WS potential has been widely used in describing nuclear processes. The recent application of the interaction to low-dimension systems has equally been successful (Aytekin et al., 2013; Aziz Aghchegala et al., 2011; Costa et al., 1999; Lu et al., 2011; Xie, 2009a, 2009b), hence the motivation for the present application to QHE. An advantage of the more realistic WS interaction is the interaction width L which mimics the wall of the classical heat engine is well defined and explicitly parameterized unlike the case of the well-studied oscillator interaction. To validate the derived Carnot's efficiency of the Woods-Saxon WS model in Eq. (33), the present result is compared with earlier works which similarly modelled the Carnot's engine using the free particle and Pöschl-Teller interactions within appropriate limits (Abe, 2011; Bender et al., 2000; E. Oladimeji et al., 2021). From Eq. (34), depending on the relative values of L_1^2 and L_3^2 , it is observed that the factor $(\alpha - 1)/(\beta - 1)$ may be greater or lesser than one (i.e., $\alpha > \beta$ or $\alpha < \beta$ respectively). Thus, giving the lower and upper limits of the possible efficiency. However, considering the order of magnitude of α and β i.e. ($\alpha \gg 1$ and $\beta \gg 1$), it is safe to assume that the factor $(\alpha - 1)/(\beta - 1) \sim 1$, hence,

$$\eta = 1 - \frac{9L_1^2}{4L_3^2} \tag{35}$$

We note also that Eq. (35) agrees with the result for free particle model in which the depth $V_o = 0$. Substituting Equ. (6) and (19) into (35), generates an efficiency

$$\eta = 1 - \frac{E_C}{E_H} \tag{36}$$

which is analogous to the classical Carnot's efficiency since $E_C \cong T_C$ and $E_H \cong T_H$. (Bender et al., 2000; E. Oladimeji et al., 2021).

4. Conclusion

In this work, we have shown explicitly that the WS potential can successfully be used in modeling the nonlinearities of a QHE. We derived the efficiency of a cyclic engine using the Eigen energies of a non-linear quantum system described by the Wood-Saxon WS potential model. The cycles are shown to be analogous to their respective classical isothermal and adiabatic processes of the Carnot cycle and the efficiency obtained with the WS model is found to agree with existing results within appropriate limits.

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