THE PÖSCHL-TELLER LIKE DESCRIPTION OF QUANTUM-MECHANICAL CARNOT ENGINE.

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ABSTRACT

In this work, an example of a cyclic engine based on a quantum-mechanical properties of the strongly non-linear quantum oscillator described by the Pöschl-Teller [PT] model is examined. Using the [PT] model as shown in our earlier works [1–4], a quantum-mechanical analog of Carnot cycle (i.e quantum heat engine) has been constructed through the changes of both, the width \(L\) of the well and its quantum state. This quantum heat engine has a cycle consisting of adiabatic and isothermal quantum processes. The efficiency of the quantum engine based on the Pöschl-Teller-like potential is derived and it’s analogous to classical thermodynamic engines.

Keywords: Quantum Thermodynamics, Quantum Mechanics, Carnot cycle, Quantum Heat Engines, Nano-Engines.

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1. INTRODUCTION

With the rapid development of quantum thermodynamics, research on quantum heat engines has become a subject of renewed interest. Of recent, diverse efforts have been made to understand the working mechanism of Quantum heat engines (QHE) [5–11] which has led to the introduction of several Quantum analogues [12–15]. These Quantum heat engines (QHE) are microscopic engines that are described by dynamical equations of motion that obey the laws of quantum mechanics [16]. This field considers analogies between quantum systems and macroscopic engines, with an example in the proposed model by Bender et al [17] of a cyclic engine based on a single quantum mechanical particle of mass \(m\) confined in an infinite one-dimensional potential well of width \(L\) (free particle [FP] in the box). This model replaces the role of piston in a cylinder and temperature in classical thermodynamics to the walls of the confining potential and energy as given by the pure-state expectation value of the Hamiltonian in Quantum thermodynamics respectively. This concept was useful in our earlier work where we formatted and applied the Pöschl-Teller [PT] potential in Joule-Brayton and Otto cycle [1–4], rather than the (free particle [FP] in the box) as used by Bender et al [17].

In this paper, we use the [PT] model to construct an adiabatic and isothermal quantum analogous process in order to analyze the efficiency of an idealized reversible heat engine i.e. Carnot engine. This model uses the walls of the containing potential to play the role of the piston in a cylinder containing an ideal gas and then constructs quantum mechanical equivalents of isothermal and adiabatic processes. The pressure \(P\) exerted on this wall as defined by Hellman and Feynman [1,4,18,19] is:

\[
P_n(L) = -\frac{\partial E_n}{\partial L}
\]
where E is the energy operator such that the formal relation between pressure P and energy E operator or Hamiltonian is $\hat{P}(\hat{x}, \hat{p}, L) = -(\partial / \partial L)H(\hat{x}, \hat{p}, L)$. The energy spectrum replaces the role of temperature which is derived from the expectation value of the Hamiltonian.

G. Pöschl and E. Teller introduced a model that is a family of anharmonic [PT]-potential $V(x; L) = -V(x; L) = V_0 \tan^{2}[\alpha(L)x]$; $\alpha(L) = \pi / L$ where $x = \pm L$, the potential becomes singular, which physically means the presence of a pair of impenetrable walls. This potential allows the exact solution of one-dimensional Schrödinger equation with fully discrete positive energy levels in the coordinate $E_n(L) > 0$ [20].

$$E_n^{PT}(L) = W(L)[n^2 + \lambda(L)(2n + 1)] \tag{2}$$

where; $W(L) = \pi^2 \hbar^2 / 2mL^2$ and $\lambda(L) = [(2/(\pi \zeta(L))^2 + 1)^{1/2} - 1$ as defined in [1].

Since the pressure operator $P_n(L) = (s/L)E_n(L)$, where $s = 2$ therefore;

$$P_n^{PT}(L) = \frac{2W(L)}{L} [n^2 + 2\lambda(L)(n + \frac{1}{2})(1 - \mu(L))] \tag{3}$$

where; $\mu(L) = 1 - [\lambda(L) - 1][2\lambda(L) - 1]^{-1}$.

2. THE CARNOT CYCLE

The classical Carnot cycle is composed of two isothermal and two adiabatic processes (see Fig.1) each of which is reversible.

Carnot cycle is the most efficient heat engine cycle allowed by physical laws. As proposed by Carnot, it’s an ideal mathematical model of a heat engine with an efficiency of almost 100%, it’s cyclic and also reversible although it’s practically impossible in real engines.

To achieve a quantum description of the Carnot cycle, Bender et al. formulated a two-state model of a single particle confined in a one-dimensional infinite potential well and have devised a reversible cycle by changing the potential width and the quantum state which shows the possibility to construct a quantum-mechanical analog of the Carnot engine [17]. In this description, the cylinder in classical Carnot cycle is replaced by a potential well in quantum Carnot cycle likewise, the fluid (an ideal gas) and temperature $T$ in classical thermodynamics is replaced with a single quantum particle and expectation value of the Hamiltonian $E$.

Classically, the temperature $T$ and internal energy of the gas in the cylinder remains constant during an isothermal process even as the piston compresses or expands the gas, work is done yet the system remains equilibrium all through. While quantumly, given that the system at the initial state $\psi(x)$ of volume $L$ is
linear combination of eigenstates $\phi_n(x)$, the expectation value of the Hamiltonian remains constant as the walls of the well moves. The expansion coefficient $a_n$ changes such that $E(L)$ remains fixed as $L$ changes:

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

(5)

where $E_n$ is the [PT] energy spectrum (1) and the coefficients $|a_n|^2$ are constrained by the normalization condition $\sum_{n=1}^{\infty} |a_n|^2 = 1$.

**Process 1: Isothermal Expansion**

Given that the piston expands isothermally such that the system is excited from its initial state $n = 1$ at point 1 (i.e. from $L = L_1$ to $L = L_2$) and into the second state $n = 2$, keeping the expectation value of the Hamiltonian constant. Thus, the state of the system is a linear combination of its two energy eigenstates:

$$\psi_n = a_1(L)\phi_1(x) + a_2(L)\phi_2(x),$$

where $\phi_1$ and $\phi_2$ are the wave functions of the first and second states respectively.

$$\psi_n = a_1(L)\sqrt{2/L} \sin(ax) + a_2(L)\sqrt{2/L} \sin(2ax)$$

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

The coefficients satisfy the condition $|a_1|^2 + |a_2|^2 = 1$. The expectation value of the Hamiltonian in this state as a function of $L$ is calculated as $E = \langle \psi | H | \psi \rangle$:

$$E(L) = W(L)[4 + 5\lambda(L) - (3 + 2\lambda(L))|a_1|^2].$$

(6)

$$E(L) = \frac{\pi^2 \hbar^2}{2mL^2} [4 + 5\lambda(L) - (3 + 2\lambda(L))|a_1|^2].$$

(7)

Setting the expectation value to be equal to $E_H$ i.e. $n = 1$

$$\frac{\pi^2 \hbar^2}{2mL_1^2} [1 + 3\lambda(L)] = \frac{\pi^2 \hbar^2}{2mL^2} [4 + 5\lambda(L) - (3 + 2\lambda(L))|a_1|^2]$$

$$L^2 = \frac{L_1^2}{[1+3\lambda(L)]} [4 + 5\lambda(L) - (3 + 2\lambda(L))|a_1|^2]$$

(8)

The max value of $L$ is when $L = L_2$ and this is achieved in the isothermal expansion when $|a_1|^2 = 0$. Therefore, from equ. (8)

$$L_2^2 = L_1^2 \frac{4 + 5\lambda(L)/1 + 3\lambda(L)}
Thus;

\[ L_2 = L_1 \left[ 4 + 5\lambda(L)/1 + 3\lambda(L) \right]^{1/2} \]  (9)

The pressure during the isothermal expansion is:

\[ P(L) = \sum_{n=1}^{\infty} (|a_1|^2 + |a_2|^2)P_n = |a_1|^2P_1 + |a_2|^2P_2 \]

\[ P_1(L) = (2W(L)/L)[4 + 5\lambda(L)\{1 - \mu(L)\} - (3 + 2\lambda(L)\{1 - \mu(L)\})|a_1|^2] \]

Considering the value \( \{1 - \mu(L)\} \) to be negligible;

\[ P_1(L) = (2W(L)/L)[4 + 5\lambda(L) - (3 + 2\lambda(L))|a_1|^2] \]  (10)

Substituting (9) into (10);

\[ \left[ 4 + 5\lambda(L) - (3 + 2\lambda(L))|a_1|^2 \right] = \frac{L^2}{L_1^2} [1 + 3\lambda] \]

Therefore;

\[ P_1(L) = \frac{\pi^2 \hbar^2}{mL_1^2} [1 + 3\lambda] \]  (11)

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

**Process 2: Adiabatic Expansion**

Next, the system expands adiabatically from \( L = L_2 \) until \( L = L_3 \). During this expansion, the system remains in the second state \( n = 2 \) as no external energy comes into the system and the change in the internal energy equals to the work performed by the walls of the well. The expectation value of the Hamiltonian is:

\[ E_L = \frac{\pi^2 \hbar^2}{2mL_3^2} [4 + 5\lambda(L)] \]

\[ E_C = 2W(L)[4 + 5\lambda(L)] \]  (12)

The pressure \( P \) as a function of \( L \) is:

\[ P_2 = \frac{2W(L)}{L} [4 + 5\lambda(L)\{1 - \mu(L)\}] \]  (13)

\[ P_2 = \frac{\pi^2 \hbar^2}{mL_3^2} [4 + 5\lambda(L)\{1 - \mu(L)\}] \]
The product $L^3 P_2(L)$ in (13) is a constant and it’s considered as the quantum analogue of the classical adiabatic process.

**Process 3: Isothermal Compression**

The system is in the second state $n = 2$ at point 3 and it compresses Isothermally to the initial (ground) state $n = 1$ (i.e. from $L = L^3$ until $L = L^4$) as 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 $\phi_1$ and $\phi_2$ are the wave functions of the first and second states respectively.

$$\Psi_n = b_1(L)\sqrt{2/L}\sin(\alpha x) + b_2(L)\sqrt{2/L}\sin(2\alpha x)$$

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

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

$$E(L) = W(L)[1 + 3\lambda(L) + (3 + 2\lambda(L))|b_2|^2] \quad (14)$$

$$E(L) = \frac{\pi^2h^2}{2mL^2} \left[ 1 + 3\lambda(L) + (3 + 2\lambda(L))|b_2|^2 \right] \quad (15)$$

Setting the expectation value to be equal to $E_L$, i.e. $n = 2$

$$\frac{\pi^2h^2}{2mL_3^2} \left[ 4 + 5\lambda(L) \right] = \frac{\pi^2h^2}{2mL^2} \left[ 1 + 3\lambda(L) + (3 + 2\lambda(L))|b_2|^2 \right]$$

$$L^2 = \frac{L_3^2}{[4 + 5\lambda(L)]} \left[ 1 + 3\lambda(L) + (3 + 2\lambda(L))|b_2|^2 \right] \quad (16)$$

The max value of $L$ is when $L = L_4$ and this is achieved in the isothermal expansion when $|b_2|^2 = 0$. Therefore, from equ. (8)

$$L_4^2 = L_3^2 [1 + 3\lambda(L)/4 + 5\lambda(L)]$$

Thus;

$$L_4 = L_3 \left[ 1 + 3\lambda(L)/4 + 5\lambda(L) \right]^{1/2} \quad (17)$$

The pressure during the isothermal compression is:
The Pöschl-Teller Like Description of Quantum Mechanical Carnot Engine

\[ P_3(L) = \frac{\pi^2 \hbar^2}{mL^3} [4 + 5\lambda] \]  

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

**Process 4: Adiabatic Compression**

The system returns to the initial state \( n = 1 \) at point 4 as it compresses adiabatically (i.e. from \( L = L_4 \) until \( L = L_1 \)). The expectation of the Hamiltonian is given by:

\[ E_H = \frac{\pi^2 \hbar^2}{2mL^2} [1 + 3\lambda(L)] \]

\[ E_H = 2W(L)[1 + 3\lambda(L)] \]  

and the pressure applied to the potential well’s wall \( P \) as a function of \( L \) is:

\[ P_A(L) = \frac{\pi^2 \hbar^2}{mL^3_1} [1 + 3\lambda(L)[1 - \mu(L)]] \]

\[ P_A(L) = \frac{2W(L)}{L} [1 + 3\lambda(L)[1 - \mu(L)]] \equiv P_1(L) \]  

The work \( W \) performed by the quantum heat engine during one closed cycle, along the four processes described above is the area of the closed loops represented in the *Fig.1*. By using eqs. (11), (13), (18) and (19) one obtains

\[ W = W_{12} + W_{23} + W_{34} + W_{41} \]

\[ W = \int_{L_1}^{L_2} P_1 dL + \int_{L_2}^{L_3} P_2(L) dL + \int_{L_3}^{L_4} P_3 dL + \int_{L_4}^{L_1} P_4(L) dL \]

Recall that;

\[ L_2 = L_1[4 + 5\lambda(L)/1 + 3\lambda(L)]^{1/2} \]

\[ L_4 = L_3[1 + 3\lambda(L)/4 + 5\lambda(L)]^{1/2} \]

Therefore;

\[ W = \int_{L_1}^{L_2} \frac{\pi^2 \hbar^2}{mL^2_1} [1 + 3\lambda]dL + \int_{L_1}^{L_3} \frac{\pi^2 \hbar^2}{mL^3_1} [4 + 5\lambda(L)[1 - \mu(L)]]dL \]

\[ + \int_{L_3}^{L_4} \frac{\pi^2 \hbar^2}{mL^2_3} [4 + 5\lambda]dL + \int_{L_4}^{L_1} \frac{\pi^2 \hbar^2}{mL^3_3} [1 + 3\lambda(L)[1 - \mu(L)]]dL \]
\[ W = \frac{\pi^2 h^2}{mL^3} \left[ \frac{(1+3\lambda)^{3/2}}{(4+5\lambda)^{3/2}} - [1 + 3\lambda]^{3/2} [4 + 5\lambda]^{3/2} \right] - \frac{\pi^2 h^2}{mL^3} \left[ \frac{(4+5\lambda)^{3/2}}{(1+3\lambda)^{3/2}} - [1 + 3\lambda]^{3/2} [4 + 5\lambda]^{3/2} \right] \] (21)

The efficiency of the heat engine is defined to be:

\[ \eta = \frac{W}{Q_H} \] (22)

given that \( Q_H \) is the quantity of heat in the high-temperature reservoir and \( W \) is the work performed by the classical heat engine. Where \( Q_H \) is the heat engine absorbed by the potential well during the isothermal expansion in quantum engine:

\[ Q_H = \frac{\pi^2 h^2}{mL^3} \left[ \frac{(1+3\lambda)^{3/2}}{(4+5\lambda)^{3/2}} - [1 + 3\lambda] \right] \] (23)

Therefore, the efficiency \( \eta \) of a quantum heat engine as defined in (20)

\[ \eta = 1 - \frac{L_1^2}{L_3^2} \left( \frac{4+5\lambda}{1+3\lambda} \right) \] (24)

Substituting the eqs. (12) and (19) into (24), the efficiency can be written as:

\[ \eta = 1 - \frac{E_C}{E_H} \] (25)

Note that this efficiency is analogous to that of a classical thermodynamic Carnot cycle.

3. OUR RESULT

The derived efficiency in equation (24) needs to be compared with earlier works of Bender et al [17] where they examined the Carnot engine as a quantum particle in a potential well i.e. free particle [FP] in the box model. In their model, \( \lambda(L) = 0 \) at the limit [1]. Therefore, the efficiency is:

\[ \eta = 1 - 4 \frac{L_1^3}{L_3^3} \] (26)

After inserting the necessary conditions, the derived efficiency is exactly the same as in [17] which is analogous to classical Carnot cycle.

4. CONCLUSION

In this work, we showed that the Pöschl-Teller [PT] oscillator can be used as a working fluid in a quantum engine, we showed that it’s possible to construct equations that are analogous to classical adiabatic and isothermal process using the Pöschl-Teller [PT] model. We also found in this paper that the derived efficiency of the quantum Carnot cycle, is analogous to the well-known efficiency from classical thermodynamics.
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Figure 1: The schematic representation of the Carnot's cycle.