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Optimization of a Single Ion Heat Engine for Adiabatic Processe at High and Low Temperature Limits

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Abstract: A quantum Otto engine with a single ion harmonic oscillator as its working substance is studied for an adiabatic operation at high and low temperature limits. Using the universal optimization method, the heat engine is effectively optimized and found to yield better working conditions in some ranges of temperature ratios. Accordingly, the figure of merit, ψ, is found to be greater than unity in the range: $0 < \frac{\beta_2}{\beta_1} \leq 0.12$; showing that the heat engine performs better in the optimized condition than in the maximum power working condition. ψ is determined to be less than one in the range $0.12 \leq \frac{\beta_2}{\beta_1} \leq 0.35$ under the same temperature limit ; depicting that the maximum power working condition is preferred to the optimized working condition. On the other hand, in the low temperature limit, the figure of merit, ψ, is found to be greater than unity in the range $3.7 < \frac{\omega_1}{\omega_2} \leq 18$; revealing that optimized working condition is better than the maximum power working condition for the heat engine. In the same temperature limit, ψ is found to be less than one in the range $0 \leq \frac{\omega_1}{\omega_2} \leq 3.7$; showing that maximum power working condition is preferred to the optimized one. For the model of heat engine studied, in some ranges of temperature ratio, it is found to work better in the optimized condition, whereas in the other ranges it performs better under the maximum power working condition. So, it is possible to switch the engine between the two conditions depending on one's need.

Keywords: Adiabatic; figure of merit ; Heat engine ; Single

1. Introduction

Physics has many divisions that deal with different natural phenomena. Thermodynamics is one of these fields that investigates the interaction between heat and work, as well as their interconversions. Though work can be directly and fully transferred to heat, transferring heat to work requires the use of a device called a heat engine. A heat engine's three crucial elements are the working matter, the operating cycle, and the energetic that regulate the operation cycle. Efficiency is one of the energetics of a heat engine which quantifies how much useful work is extracted from a given amount of input heat, and it is the ratio of total work done by the heat engine to heat energy flowing into it from the hot reservoir [1]. It became a fundamental topic of thermodynamics when Sadi Carnot calculated the maximum efficiency of a reversible heat engine in 1824 [2]. Carnot was a pioneer in proposing the concept of efficiency. However, heat engines with Carnot efficiency require qua-static processes that take an infinite amount of time to complete a unit cycle. But, such extremely slow processes have no practical power output [3]. To overcome this problem, RS. Berry *et al*. developed Finite Time Thermodynamics (FTT) [4]. Following the invention of FTT in 1975, Curzon and Ahlborn reported the efficiency of a heat engine that went through a Carnot-like loop at maximum power, and their work contributed to the recognition of FTT[5]. They verified that, unlike the Carnot engine, such a heat engine produces nonzero power output [6]. Since then, several studies have been conducted on various models of heat engines in order to determine their efficiency at maximum power.

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One of these was a Brownian heat engine operating in a changing harmonic potential, which Schmiedl and Seifert investigated to determine the efficiency at maximum power[7]. They showed that the heat engine works at the Carnot efficiency limit and produces zero power output. Their expression of efficiency at maximum power, on the other hand, differed from the Curzon-Ahlborn efficiency [8]. Several investigations have also been performed in the wake of Schmiedl and Seifert's work to develop a quantum model of heat engines in order to construct miniaturized devices that utilize energy resources at the microscopic scale [9]-[10]. Quantum heat engines are excellent model systems for understanding the formation of fundamental thermodynamic descriptions at the microscopic level. It also describes briefly the connection of classical and quantum thermodynamic systems [11]. One of the investigations devoted to develop models of quantum heat engines was a quantum Otto cycle for a harmonic oscillator [12]. The study developed a quantum Otto engine model , which is a quantum generalization of the two adiabats and two isochores of a typical four-stroke car engine [13]-[15]. A recent publication described an optimization study of a quantum Otto engine whose working substance is a two-atomic system [16]. However, the applicability of this research to the Otto engine, which employs various kinds of quantum systems rather than two atomic-systems, raises an intriguing question that merits more exploration. To deal with this problem, the researchers developed a quantum Otto engine model with two isochores and two adiabats processes using a single ion and a harmonic system working substance [17]. Recent research has shown that the efficiency at maximum power (EMP) of this heat engine corresponds to the Curzon-Ahlborn result for an adiabatic process [18]. Running at maximum power, however, wastes a substantial amount of the input energy[19]. Hence, there must be a question of how to make a trade-off between maximum efficiency and maximum power of the heat engine using a universal optimization method.

2. Model and methods

2.1. Model of the Heat engine

A model of quantum Otto engine whose working substance is a single ion harmonic oscillator with a modulating frequency of ω_t, is considered. The frequency of the oscillator changes over time and switches between ω_1 and ω_2. The engine uses the quantum Otto cycle and has four different stages, as seen in **Fig. 1**.

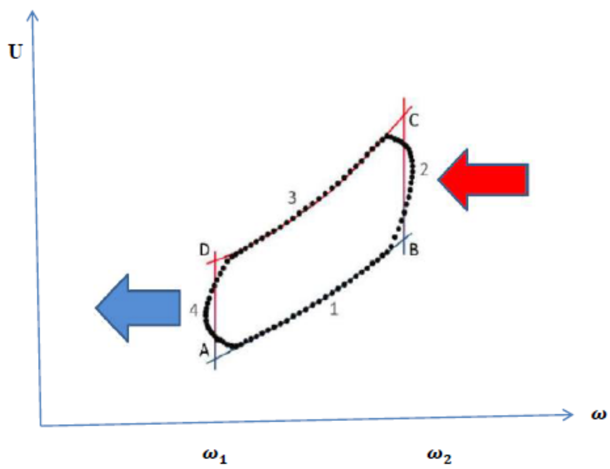

Figure 1. Energy-frequency diagram of a single ion heat engine

1. Isentropic compression, $A(\omega_1, \beta_1) \rightarrow B(\omega_2, \beta_1)$ **:** While the system is isolated, the frequency is modulated over time $\mathbf{t_1}$. The oscillator's entropy is not varying with time since the evolution is single.

2. Hot isochore, $B(\omega_2, \beta_1) \rightarrow C(\omega_2, \beta_2)$ **:** At a fixed frequency, the oscillator is weakly linked to a reservoir at inverse temperature β_2 and allowed to relax to the thermal state C at time $\mathbf{t_2}$.
3. Isentropic expansion, $C(\omega_2, \beta_2) \rightarrow D(\omega_1, \beta_2)$**:** During time $\mathbf{t_3}$, the frequency is reset to its initial value. At constant entropy, the isolated oscillator develops unitarily toward the non-thermal state D.
4. Cold isochore, $D(\omega_1, \beta_2) \rightarrow A(\omega_1, \beta_1)$**:** The system is poorly linked to a reservoir during $\mathbf{t_4}$ and soon relaxes to its initial thermal state. The frequency is maintained steady once more.

From the model, the mean energy of the oscillator is varying from one stroke to the other while the frequency of oscillator is varied. Hence, the model of heat engine can be taken as canonical ensemble whose energy varies. The quantum mechanical condition is used to calculate the energy eigenvalues of a one-dimensional quantum harmonic oscillator [20], and are given by

$$E_n = (n + \frac{1}{2})\hbar\omega, \qquad n = 0, 1, 2, 3, ... \tag{1}$$

For a single oscillator, the partition function, $Q_1(\beta)$, is given by

$$Q_1(\beta) = \sum_0^{\infty} e^{-\beta E_n}. \tag{2}$$

The partition function for the heat engine is obtained by employing Equation (1) into Equation (2).

$$Q_1(\beta) = \left(e^{\frac{1}{2}\beta\hbar\omega} - e^{-\frac{1}{2}\beta\hbar\omega}\right)^{-1}. \tag{3}$$

The mean quantum energies, U, of the oscillators during the four phases of the cycle for the adiabatic process (where the modulating frequencies of the oscillator are quasi-statically changed) are calculated using Equation (3), and are given by:

$$U_A = \frac{\hbar\omega_1}{2} \coth\left(\frac{\beta_1\hbar\omega_1}{2}\right), \tag{4}$$

$$U_B = \frac{\hbar\omega_2}{2} \coth\left(\frac{\beta_1\hbar\omega_1}{2}\right), \tag{5}$$

$$U_C = \frac{\hbar\omega_2}{2} \coth\left(\frac{\beta_2\hbar\omega_2}{2}\right), \tag{6}$$

and

$$U_D = \frac{\hbar\omega_1}{2} \coth\left(\frac{\beta_2\hbar\omega_2}{2}\right). \tag{7}$$

No work is done during the second and fourth strokes as isochoric processes are involved. However, there is mean work done by system during the first and the third strokes since the heat engine is operating adiabatically. The mean work done during the first and third strokes are, respectively given by:

$$W_1 = U_B - U_A = \left[\frac{\hbar\omega_2}{2} - \frac{\hbar\omega_1}{2}\right] \coth\left(\frac{\beta_1\hbar\omega_1}{2}\right), \tag{8}$$

and

$$W_3 = U_D - U_C = \left[\frac{\hbar\omega_2}{2} - \frac{\hbar\omega_2}{2}\right] \coth\left(\frac{\beta_1\hbar\omega_2}{2}\right). \tag{9}$$

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The heat energy supplied into the heat engine from the hot reservoir during the second stroke and the heat energy discharged from the heat engine to the cold reservoir during the fourth stroke are, respectively given by:

$$Q_2 = U_C - U_B = \frac{\hbar\omega_2}{2}\left[\coth\left(\frac{\beta_2\hbar\omega_2}{2}\right) - \coth\left(\frac{\beta_1\hbar\omega_1}{2}\right)\right], \tag{10}$$

and

$$Q_4 = U_A - U_D = \frac{\hbar\omega_1}{2}\left[\coth\left(\frac{\beta_1\hbar\omega_1}{2}\right) - \coth\left(\frac{\beta_2\hbar\omega_2}{2}\right)\right]. \tag{11}$$

The power and efficiency of a heat engine are its two most important qualities.. Power output is the rate of change of total work done per-cycle, and is given by:

$$P = -\frac{(W_1 + W_3)}{T}. \tag{12}$$

,where $T = t_1 + t_2 + t_3 + t_4$, is the total amount of time spent relaxing. For high temperature regime, $\frac{\beta_i\hbar\omega_i}{2} \ll 1$. Hence, using Taylor's series expansion, $\coth\left(\frac{\beta_i\hbar\omega_i}{2}\right) \approx \frac{2}{\beta_i\hbar\omega_i}$. The power output of the heat engine, at its classical limit, calculated by employing Equations (8) and (9) into Equuation (12), and given by

$$P = -\frac{1}{\tau}\left(\frac{\omega_2}{\beta_1\omega_1} - \frac{1}{\beta_1} + \frac{\omega_1}{\beta_2\omega_2} - \frac{1}{\beta_2}\right). \tag{13}$$

The efficiency of a heat engine is denoted by η, and it is the ratio of total work done by the heat engine to heat energy flowing into it from the hot reservoir.

$$\eta = -\frac{(W_1 + W_2)}{Q_2} \tag{14}$$

The efficiency of the heat engine at high temperature limit is calculated by inserting Equations (8), (9), and (10) into this equation, and is given by

$$\eta = 1 - \frac{\omega_1}{\omega_2}. \tag{15}$$

The maximum power of the heat engine is obtained by differentiating Equation (14) with respect to ω_2.

$$P_{max} = -\frac{1}{\tau}\left(\frac{2\beta_1\beta_2 - \sqrt{\beta_1\beta_2}(\beta_1 + \beta_2)}{\beta_1\beta_2\sqrt{\beta_1\beta_2}}\right). \tag{16}$$

The corresponding efficiency at maximum power for the heat engine at high temperature regime is given as

$$\eta_{maxP} = 1 - \sqrt{\frac{\beta_2}{\beta_1}}. \tag{17}$$

Equation (17) indicates that the efficiency at maximum Power (EMP) for a single ion heat engine coincides to the Curzon-Ahlborn finding, for a sudden switching frequency of oscillators, at the classical limit.

For low temperature regime, where $\beta_1\hbar\omega_1 \gg 1$ and $\beta_2\hbar\omega_2 \ll 1$, $\coth\left(\frac{\beta_1\hbar\omega_1}{2}\right) = 1$ and $\coth\left(\frac{\beta_2\hbar\omega_2}{2}\right) \approx \frac{2}{\beta_2\hbar\omega_2}$. Then, using these conditions, the power and efficiency of the heat engine, at low temperature limit, are given by:

$$P = -\frac{1}{\tau}\left[\frac{\hbar}{2}(\omega_2 - \omega_1) + \frac{\omega_1}{\beta_2\omega_2} - \frac{1}{\beta_2}\right], \tag{18}$$

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and

$$\eta = 1 - \frac{\omega_1}{\omega_2}. \tag{19}$$

Following the same steps, gives the maximum power and the corresponding efficiency at maximum power for the heat engine at low temperature limit, respectively as

$$P_{max} = -\frac{1}{\tau}\left[\frac{4\sqrt{\hbar\omega_1} - \sqrt{2\beta_2}\left(\hbar\omega_1 - \frac{1}{\beta_2}\right)}{2\sqrt{2\beta_2}}\right], \tag{20}$$

and

$$\eta_{maxP} = 1 - \sqrt{\frac{\hbar\omega_1\beta_2}{2}}. \tag{21}$$

3. Techniques of optimization

The optimization approach proposed by A. C Hernandez *etal*. was utilized in this study to find the optimal balance between maximum efficiency and maximum power of the heat engine. A. C Hernandez *et al*. proposed an objective function that provides the optimal balance of usable energy and lost useful energy [21]. Their method applies to all types of heat engines. They developed the objective function, Ω, which is given by

$$\Omega = (2\eta - \eta_{max} - \eta_{min})P_i. \tag{22}$$

, where η is the efficiency, η_{max} is the maximum efficiency, η_{min} is the minimum efficiency and $P_i = \frac{Q_2}{\tau}$ is the input power of the heat engine. This paper used equation (22) to make optimization between maximum efficiency and maximum power of a single ion heat engine for adiabatic operation at classical limit. First, the developed objective function of the heat engine was optimized in terms of the parameter(s) of the heat engine. Next, the optimized quantities and scaled quantities of the heat engine were calculated. Finally, the figure of merit, a quantity that determines the overall performance of the heat engine, was determined. If the figure of merit is greater than unit, the heat engine better operates in the optimum working condition, and if it is less than one, it better performs in maximum power working condition [22].

4. Result and Discussion

The case where the maximum efficiency is one (Carnot efficiency when the temperature of the hot reservoir is much greater than that of the cold reservoir) and the minimum efficiency is zero (Carnot efficiency when the two reservoirs are in thermal equilibrium with each other) was used to find the objective function for the heat engine in this work. Equation (22) was used to calculate the heat engine's objective function, at both temperature limits. For high temperature limit, the objective function of the heat engine is calculated and given by

$$\Omega = \left(1 - 2\frac{\omega_1}{\omega_2}\right)\left(\frac{\beta_1\omega_1 - \beta_2\omega_2}{\tau\beta_1\beta_2\omega_1}\right). \tag{23}$$

Optimizing the objective function, Ω, with respsect to ω_2, gives optimized power and optimized efficiency of the heat engine, respectively, for an adiabatic process at high temperature limit.

$$P_{opt} = -\frac{1}{\tau}\left(\frac{3\sqrt{\beta_1\beta_2} - (\beta_1 + \beta_2)\sqrt{2}}{\beta_1\beta_2\sqrt{2}}\right). \tag{24}$$

and

$$\eta_{opt} = 1 - \sqrt{\frac{\beta_2}{2\beta_1}}, \tag{25}$$

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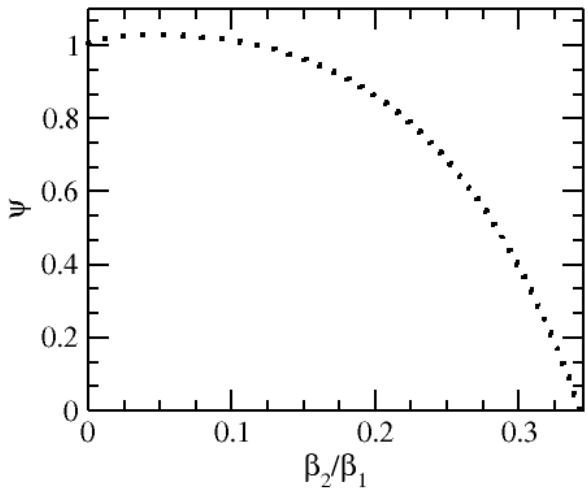

Figure 2. Plot of figure of merit versus $\frac{\beta_2}{\beta_1}$ for high temeprature regime

In the present work, a scaled quantity is the ratio of the optimized quantity to the maximum quantity or the quantity at maximum power [22]. Hence, employing Equations (16), (17), (24) and (25) gives the scaled quantities of the heat engine at high temeprature limit, respectively as

$$P_{scaled} = \frac{3\beta_2 - \beta_1\sqrt{\frac{2\beta_2}{\beta_1}}\left(1+\frac{\beta_2}{\beta_1}\right)}{2\sqrt{2}\beta_2 - \beta_1\sqrt{\frac{2\beta_2}{\beta_1}}\left(1+\frac{\beta_2}{\beta_1}\right)}, \tag{26}$$

and

$$\eta_{scaled} = \frac{1-\sqrt{\frac{\beta_2}{2\beta_1}}}{1-\sqrt{\frac{\beta_2}{\beta_1}}}. \tag{27}$$

The figure of merit, ψ, is a number that describes the overall performance of a heat engine [22]. It is defined as the product of scaled power and scaled efficiency of the heat engine. Hence, the figure of merit of the heat engine, ψ, at high temperature limit and for adiabatic operation is determined by using equations (26) and (27).

$$\psi(\beta_1,\beta_2) = \frac{-2\frac{\beta_2^2}{\beta_1^2} + \frac{\beta_2}{\beta_1}\left(5\sqrt{\frac{\beta_2}{\beta_1}} - 4\sqrt{2}\right) + 2\sqrt{\frac{\beta_2}{\beta_1}}}{-2\frac{\beta_2^2}{\beta_1^2} + 6\frac{\beta_2}{\beta_1}\left(\sqrt{\frac{\beta_2}{\beta_1}} - 1\right) + 2\sqrt{\frac{\beta_2}{\beta_1}}}. \tag{28}$$

Using Equation (28), the plot of ψ versus $\frac{\beta_2}{\beta_1}$ is plotted within the interval $0 < \frac{\beta_2}{\beta_1} \leq 0.35$ as shown in **Fig.** 2.

As it can be seen from the plot, the figure of merit is increasing as $\frac{\beta_2}{\beta_1}$ increases from zero to 0.0117, at which it becomes maximum. Then, it starts to decrease afterward for the remaining ratio of the two temperature values. Even though it is starts to decrease from this point, the figure of merit remains greater than one in the range: $0 < \frac{\beta_2}{\beta_1} \leq 0.12$, in which the heat engine performs best under the optimized working condition. For the range $0.12 < \frac{\beta_2}{\beta_1} \leq 0.35$, the figure of merit is not only decreasing with the temperature ratios, but it is also less than one in which the heat engine performs its task in the maximum power working condition.

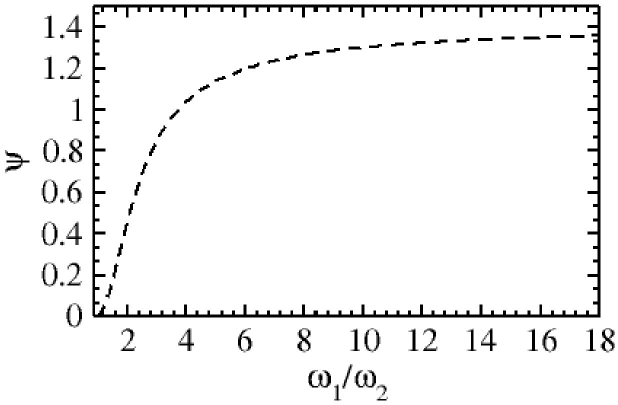

Figure 3. Plot of figure of merit versus $\frac{\omega_1}{\omega_2}$ for high low regime

For low temperature limit, the objective fuction of the heat engine is calculated and is given by

$$\Omega = \left(1 - 2\frac{\omega_1}{\omega_2}\right)\left(\frac{2 - \beta_2\hbar\omega_2}{2\tau\beta_2}\right). \tag{29}$$

Optimizing the objective function, Ω, with respsect to ω_2 gives the optimized power and the corresponding optimized efficiency of the heat engine, for an adiabatic process at low temperature limit, respectively as

$$P_{opt} = -\left[\frac{3\sqrt{\beta_2\hbar\omega_1} - (\beta_2\hbar\omega_1 + 1)}{2\tau\beta_2}\right], \tag{30}$$

and

$$\eta_{opt} = 1 - \sqrt{\frac{\beta_2\hbar\omega_1}{4}}. \tag{31}$$

The scaled quantities of the heat engines at low temeprature limit can be obtained by employing equations (20) (21) (30) and (31), which are given by

$$P_{scaled} = \frac{3\sqrt{2}(\sqrt{\beta_2\hbar\omega_1} - \beta_2\hbar\omega_1 - 1)}{4\sqrt{2\beta_2\hbar\omega_1} - 2\beta_2\hbar\omega_1 + 2}, \tag{32}$$

and

$$\eta_{scaled} = \frac{2\sqrt{2} - \sqrt{2\beta_2\hbar\omega_1}}{2\sqrt{2} - \sqrt{\beta_2\hbar\omega_1}}. \tag{33}$$

The figure of merit for the heat engine at low temperature limit is the product of equations (32) and (33) and is given by

$$\psi(\omega_1, \omega_2) = \frac{4\sqrt{2}\frac{\omega_1^3}{\omega_2^3} - \left(6 + 4\sqrt{2}\right)\frac{\omega_1^2}{\omega_2^2} + 7\frac{\omega_1}{\omega_2} - 1}{4\sqrt{2}\frac{\omega_1^3}{\omega_2^3} - 4\sqrt{2}\frac{\omega_1^2}{\omega_2^2} + 7\frac{\omega_1}{\omega_2} + \sqrt{2}}. \tag{34}$$

As it can been observed from **Fig. 3**, ψ is monotonously increasing as the frequency ratio increases from small values to nearly 6, and then tends to saturate afterwards. In particular, as $\frac{\omega_1}{\omega_2}$ increases from 0 to 3.7, even though ψ is increasing, it is still less than one. This can be interpreted as the region in which the heat engine performs better in its maximum power working condition than the optimized one. Contrary to this assertion, for higher values of the frequency ratio, $3.7 < \frac{\omega_1}{\omega_2} \leq 18$, the numerical value of ψ is greater than one. Here, the heat engine yields overall performance in the optimized working condition. So, it is possible to switch values of $\frac{\omega_1}{\omega_2}$ to change one mode of operation to another(maximum power condition $\rightleftharpoons$ optimum condition).

5. Conclusions

The figure of merit of the heat engine, ψ, determines the overall performance of the heat engine, and its plot versus the parameters of the heat engine identifies the region of optimum working condition as well as that of maximum power working condition. For both temperature limits, the result depicted that working under optimum working condition is better than working at maximum power in some intervals and working at maximum power is better than working under optimum working condition in some other intervals under the plot. This indicates that, the heat engine is successfully optimized, and revealed mixed conditions (optimum working condition and maximum power working condition). So, it is possible to switch the heat engine between the two conditions depending on one's need. This study focused mainly on making the best compromise between maximum efficiency and maximum power of a single ion heat engine for an adiabatic process at high and low temperature limits. Future studies may focus on the case of non-adiabatic processes at high and low temperature limits.

Author Contributions: Both authors contributed to the research design work. The research work was conceptualized by Mr. Abdi Belina and Dr. Tolasa Adugna. Mr. Abdi performed the analytical derivation and graphical findings. Supervision is performed by Dr. Tolasa Adugna. The first draft of the manuscript is written by Mr. Abdi Belina , and the authors provided feedback on prior versions of the manuscript. The final manuscript was reviewed and approved by both authors.

Written informed consent for publication must be obtained from participating patients who can be identified (including by the patients themselves). Please state "Written informed consent has been obtained from the patient(s) to publish this paper" if applicable.

Data Availability Statement: Data sharing is not applicable since the paper presents solely theoretical research.

Conflicts of Interest: I hereby certify, on behalf of the contributors, that I have read, understood, and agreed to the submission declaration, policies, and guidelines of the journal. The article is the authors' original work, and neither it has been published before nor is it being considered for publication somewhere else. There are no disclosed conflicts of interest for the authors. I shall take full responsibility for the submission on behalf of the co-author.

The appendix is an optional section that can contain details and data supplemental to the main text—for example, explanations of experimental details that would disrupt the flow of the main text but nonetheless remain crucial to understanding and reproducing the research shown; figures of replicates for experiments of which representative data are shown in the main text can be added here if brief, or as Supplementary Data. Mathematical proofs of results not central to the paper can be added as an appendix.

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