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Estimation of optimum thermoelectric efficiency with considering single quantum dot

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ABSTRACT

In this work, the performance conditions for achieving maximum power of nano-thermodynamic engines including of single provided quantum level between two leads at different chemical potentials and pressures are determined .this model defined a unique level with resonance (i.e without broadening). This issue occurred when the quantum dot barriers are thick.
***Key words**: Electron, quantum dot, nano, efficiency*

INTRODUCTION

The "Energy Crisis" has become a major challenge in front of engineers across the globe due to rapidly increasing demands and consumption of energy. For almost two hundred years, the main energy resource has been fossil fuel and will continue to supply much of the energy for the next two and half decades. Worldwide oil consumption is expected to rise from 80million barrels per day in 2003 to 98 million barrels per day in 2015 and then to 118 million barrels per day in 2030. [1]Thermoelectric engines are all solid-state devices that convert heat into electricity. Unlike traditional dynamic heat engines, thermoelectric engines contain no moving parts and are completely silent. Such generators have been used reliably for over 30 years of maintenance-free operation in deep space probes such as the Voyager missions of NASA.[2] Compared to large, traditional heat engines, thermoelectric generators have lower efficiency. But for small applications, thermoelectric can become competitive because they are compact, simple (inexpensive) and saleable. Thermoelectric systems can be easily designed to operate with small heat sources and small temperature differences. Such small generators could be mass produced for use in automotive waste heat recovery or home co-generation of heat and electricity. Thermoelectric have even been miniaturized to harvest body heat for powering a wristwatch. A thermoelectric produces electrical power from heat flow across a temperature gradient [3]. As the heat flows from hot to cold, free charge carriers (electrons or holes) in the material are also driven to the cold end . The resulting voltage is proportional to the temperature difference via the See beck coefficient. By connecting an electron conducting (n-type) and hole conducting (p-type) material in series, a net voltage is produced that can be driven through a load. (see Fig.1)

The thermoelectric material is selected on the basis of power factor , figure of merit and melting point. In general, for studying the efficiency of nanothermoelectric engine can be used as single and two quantum dots. In the following, both of them are introduced .But the main idea of this letter is to present a detailed thermodynamic analysis of electron transport through a single quantum dot connecting two leads at different temperatures and chemical potentials.

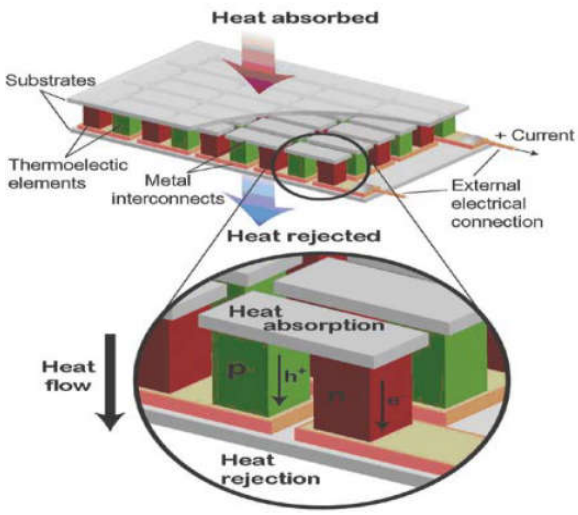


Fig1.Schematic of a thermoelectric generator*.*

Quantum dot heat engine

What are heat engines**?** Quantum dot heat engines will revolutionize thermoelectric power due to their high efficiency as compared to standard heat engines. Amazingly, the quantum dot heat engine produces as much energy per square meter as sunlight on the Earth. **How** quantum dot heat engine **works? For answering to this question see that Fig.2**

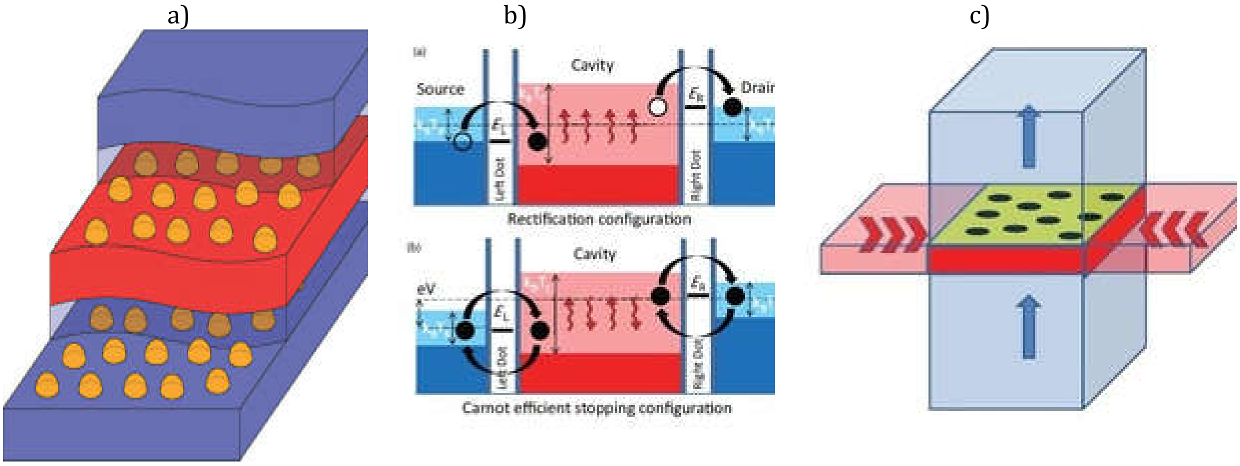


Fig2.a) Quantum Dot Heat Engine b) Energy Level Diagram c) Heat and Electron Flow Diagram

The image to the left depicts a cross section of the "Swiss Cheese Sandwich" thermoelectric generator, which facilitates the movement of electrons. The cold bottom layer is beneath a layer of QDs. This is covered by a hot central semiconductor. A fourth layer covers this with a different layer of QDs, and finally the fifth layer is a cold electrode. Pictured in the center is the energy level diagram of the quantum dot heat engine. Fig.3 is a fish ladder analogy to simplify how this works.In the figure to the right, the red arrows represent heat flow directed towards the central layer of the quantum dot heat engine. The blue arrows represent the flow of electrons through the engine. The yellow-green layer represents the resonant QD semiconductor material "swiss cheese" in between the hot and cold conductive plates. Unlike other thermoelectric engines, the quantum dot heat engine is unique in that the hot material is central, surrounded by
two cold ends.

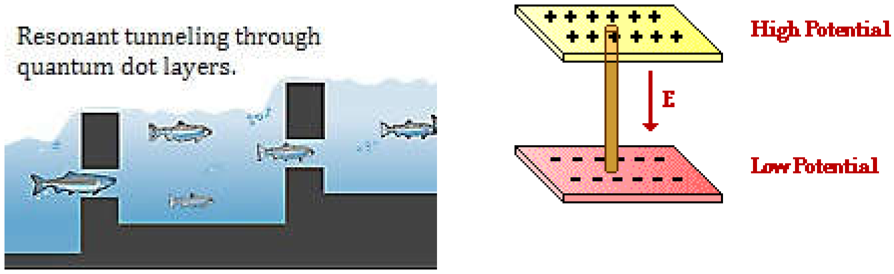


Fig.3:a fish ladder analogy

Electrons traveling through the quantum dot heat engine resemble salmon swimming up a fish ladder. The bottom cold layer of the heat engine contains electrons with various energy levels (Fermi energy spread). Once these electrons reach a certain energy level, they “jump” (called resonant tunneling) from the cold to the hot layer. Here the electrons are facilitated by a layer of resonantly-tuned quantum dots, the same way that a fish ladder helps salmon swim upstream. After gaining kinetic energy in the hot central layer of the heat engine, the process is repeated as the electrons tunnel through a second quantum dot layer from the hot layer to the top cold layer. The electrons are stored in a capacitor which is discharged to power internal medical devices.

Thermoelectric efficiency in two quantum dots connected in parallel

Quantum dots are semicoductornanocrystals that are so small. They are practically considered dimensionless. They are tiny nanocrystals that glow (to produce light and/or heat without smoke or flames) when stimulated by an external source such as Ultraviolet (UV) light. How many atoms are included in the quantum dots determines their size and the size of the quantum dot determines the color of light emitted. Quantum dots are more closely related to an atom than a bulk material because of their discrete, quantized energy level. Band gaps, depends on the relationship between the size of the crystal and the exciton Bohr radius. In the strong confinement regime the band gap is smaller where the size of the quantum dots is smaller than the excitant Bohr radius as the energy levels split up. Due to the energy level split up the emission energy becomes increases (the sum of the energy level in the smaller band gaps in the strong confinement regime is larger than the energy levels in the band gaps of the original levels in the weak confinement regime) and the emission at various wavelength. The quantum dot energy level split up to the degree that the energy spectrum is almost continuous thus the quantum dot emits white light. The smaller quantum dots have higher energy, smaller wavelength and go toward blue color and the larger quantum dots have smaller energy, higher wavelength and go toward red color shown Fig.2.1. Quantum dots can be synthesized to be essentially any size, and therefore, produce essentially any wave length. It can be made from a range of materials (2nm-10nm in diameter), currently the most commonly used materials include zinc sulphide, lead sulfide, cadmium selenide and Indium Phosphide. Many of the promising applications for quantum dots will be used within the human body [4].In the rest of this Chapter we take two quantum dots that work as thermoelectric engine and use stochastic thermodynamic method to find quantities such as current, heat flux, power, efficiency and entropy.

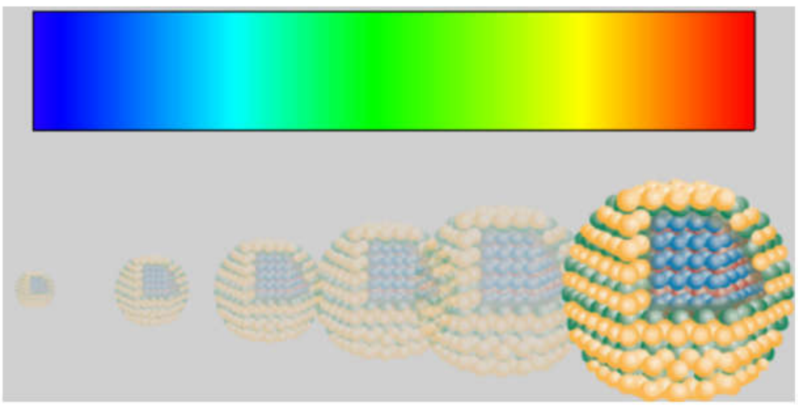


Figure 4: The size of the quantum dot corresponding with colors.

The concept of Carnot efficiency is a central cornerstone of thermodynamics. According to this principle, the efficiency, defined as the ratio of work output over heat input for a machine operating between two thermal baths at temperatures T_l and $T_r (T_r > T_l)$is at most equal to

$$\eta_c = 1 - \frac{T_l}{T_r} \quad (1)$$

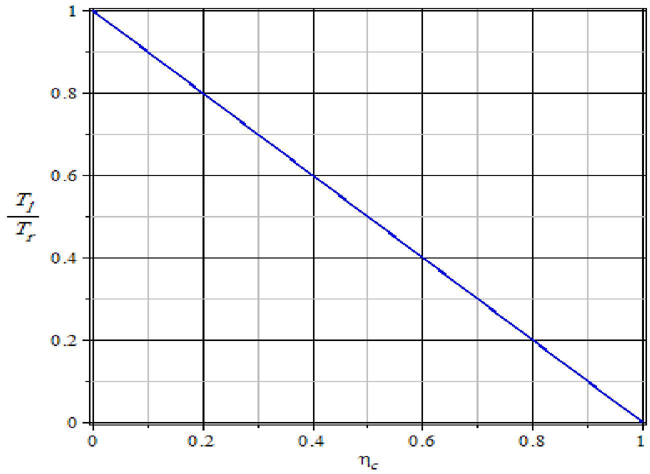


Fig.5: Variations of $\frac{T_l}{T_r}$ in terms of η_c

In figure 5 the variations of $\frac{T_l}{T_r}$ in terms of η_c is given.This is a universal result which remains valid for small-scale fluctuating systems. However, reversible processes require infinitely slow operation, implying that such engines produce zero power. In a groundbreaking paper, Curzon and Ahlborn [5] calculated this efficiency for the Carnot engine in the so-called endo-reversible approximation (taking into account the dissipation only in the heat transfer process).They found a strikingly simple formula, namely

$$\eta_{cA} = 1 - \sqrt{1 - \eta_c} \approx \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \frac{6\eta_c^3}{96} + \cdots \quad (2)$$

The field of thermoelectricity went through a revival In the early1990s due to the discovery of new thermoelectric materials with significant higher thermodynamic yields [6]. Of particular interest are the developments in the context of nanostructured materials [7]. For example, thermoelectric experiments have been reported on silicon nanowires[8],individual carbon nanotubes [9] and molecular junctions [10]. Furthermore, it has been reported that Carnot efficiency can be reached for electron transport between two leads at different temperatures and chemical potentials, by connecting them through a channel sharply tuned at the energy for which the electron density is the same in both leads[11,12].A double-barrier resonant tunneling structure has been proposed as a possible technological implementation[13].

The thermoelectric device is the simplest prototype of such systems. It consists of a quantum dot with a single resonant energy level in contact with two thermal reservoirs at different temperatures, see Fg.6.

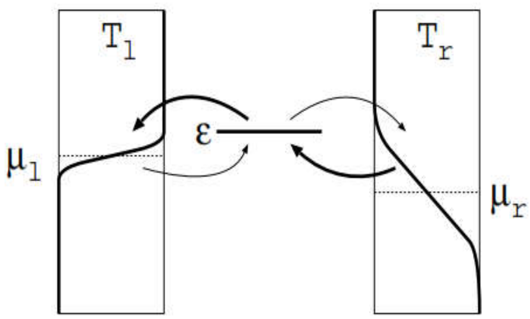


Fig.6.Sketch of the level embedded between two leads at different temperatures and chemical potentials.

Two quantum dots are connected in parallel to two (hot and cold) heat reservoirs of temperaturesT_r and T_l , respectively as shown in Fig.7. The contacts to which the quantum dots are connected have chemical potentials μ_r and μ_l as shown in the same figure.

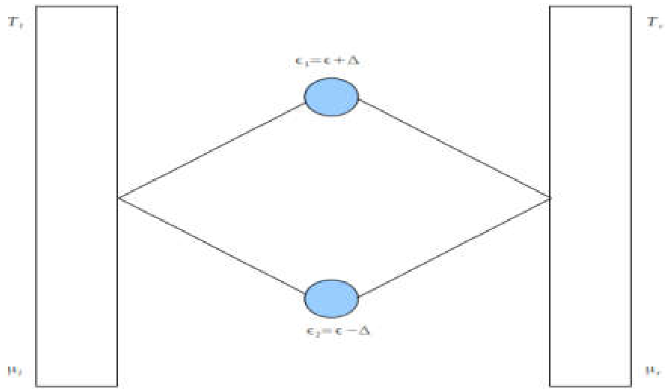


Figure 7: Sketch of nano thermoelectric engine consist of a two quantum dot embedded between two leads at different temperature and chemical potentials. We choose by convention $T_l<T_r$.

Due to their size variation, the quantum dots have different single energy levels associated with each of them. Accordingly, we consider the single energy level of the first quantum dot $\epsilon_1$to be $\epsilon + \Delta$ while that of the second quantum dot $\epsilon_2$to be $\epsilon \;\; - \Delta$. The temperature and chemical potential difference between the two contacts generate current through the two quantum dots through electron hopping to (or from) the leads to the quantum dot which is either empty or filled.We assume that the electrons thermalize instantaneously to temperature of the leads T_r (T_l) upon tunneling to the reservoirs. In order to describe the basic mechanism to produce heat and work, we assume that the energy of the level is varied in time. Upon varying the energy of the level,a certain amount of (positive or negative) energy flows into the system in the form of heat and work. If the level occupied by an electron while it is lowered (raised), power is extracted from (injected into) the system, $W < 0$($W > 0$).If the level remains empty while its energy is changed, neither power nor heat flux are produced. When the empty (filled) level at energy $\epsilon + \Delta$ and $\epsilon - \Delta$ is filled (emptied) by an electron, an amount of heat flux Q_r(Q_l) enters the system.We now turn to the mathematical analysis of the thermoelectric engine represented in fig.8. A two quantum dot, with orbital energy $\epsilon \;\; + \Delta$ and $\epsilon_1 - \Delta$, exchanges electrons with a cold left lead, temperatureT_l and chemical potential μ_l , with a hot right lead, temperatureT_r and chemical potential μ_r . The quantum dot is either empty(state 1) or filled(state 2) for the first quantum dot and the second quantum dot either empty(state 3) or filled(state 4).

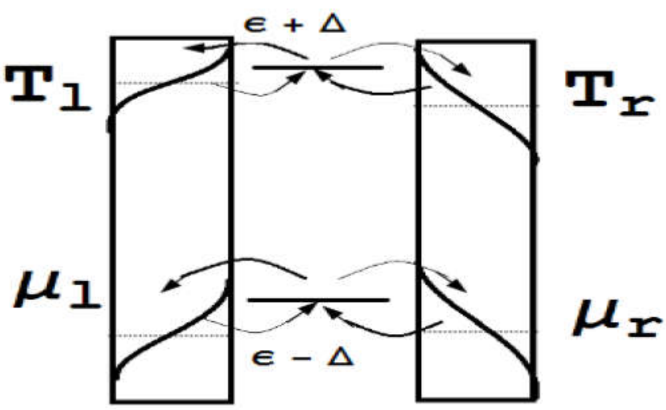
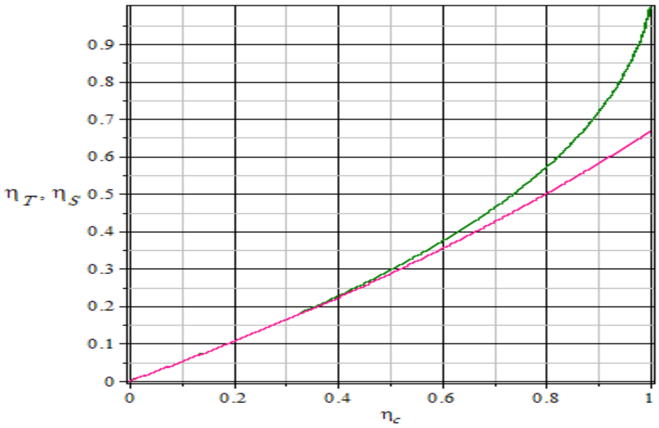


Figure 8: Sketch of nano- thermoelectric engine consist of a two quantum dot embedded between two leads at different temperature and chemical potentials. We choose by convention T_l<Tr.

Notice that in the following we consider only nanothermoelectric engine consisting of a single quantum dot.

The efficiency at maximum power was also addressed in the context of stochastic thermodynamics in[13],where it was shown that the efficiency at maximum power fora Brownian particle undergoing a

Carnot cycle through the modulation of a harmonic potential is given by $\eta_S = \frac{2\eta_c}{4-\eta_c} \approx \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \frac{3\eta_c^3}{96} + \cdots$ By an entirely different calculation, dealing with the Feynman ratchet and pawl model(which operates under steady rather than cyclic conditions),the efficiency at maximum power was found to be[14] $\eta_T = \frac{\eta_c^2}{[\eta_c-(1-\eta_c)\ln(1-\eta_c)]} \approx \frac{\eta_c}{2} + \frac{\eta_c}{8} + \frac{7\eta_c}{96} + \cdots$.All three of the above results agree, as they should[15],to linear order in η_c.Moresurprisingly,the coefficient of the quadratic term is also identical. This raises the question as to whether universality also applies to the coefficient of the quadratic term.For having a comparison between η_S and $\eta_T$see Fig.9.



.(green colorη_T:and pink color:η_S)Fig.9: Variations of η_S andη_T in terms of η_c

In particular, the efficiency at maximum power will be found to be $\approx \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + \cdots$, withthe coefficient of η_c^2again equal to $\frac{1}{8}$.

According to mathematical analysis of the thermoelectric engine(Fig.6)in which presented by M. Esposito and et al., [16],(with considering a single-level quantum dot, with orbital energy ε ,exchanges electrons with a cold left lead, temperature T_l and chemical potential μ_l, and with a hot right lead, temperature T_r and chemical potential μ_r. The quantum dot is either empty (state1) or filled (state2)) , the corresponding thermodynamic efficiency is given by

$$\eta \equiv \frac{w}{Q_r} = \frac{W}{Q_r} = \frac{\mu_l-\mu_r}{\varepsilon-\mu_r} = 1-(1-\eta_c)\frac{x_l}{x_r} \qquad (3)$$

The crucial variables of the problem are the scaled energy barriers(with k_B=1):

$$x_i = \frac{\varepsilon-\mu_i}{T_i}, \quad i = l, r \qquad (4)$$

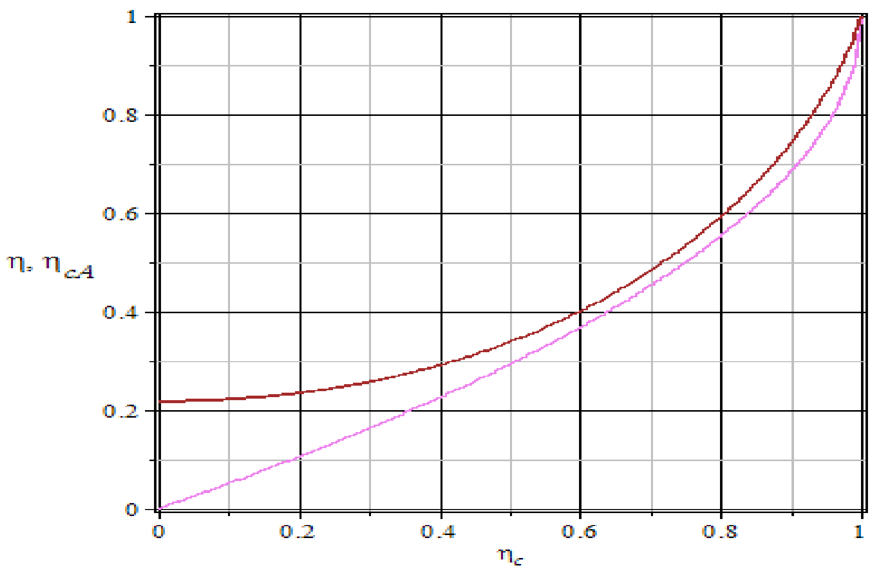
Such that from [16] we have:

$$x_l = 2\ln\left[\frac{\cosh(x_r/2)}{\sqrt{1-\eta_c}} + \sqrt{\frac{\cosh^2(x_r/2)}{1-\eta_c} - 1}\right] \qquad (5)$$

and

$$x_r - \sqrt{2}\cosh\left({}^{x_r}/_2\right)\sqrt{2\eta_c - 1 + \cosh(x_r) +} \, 2(\eta_c - 1) \times \ln\left[\frac{\cosh\left({}^{x_r}/_2\right)+\sqrt{2\eta_c-1+\cosh(x_r)}/\sqrt{2}}{\sqrt{1-\eta_c}}\right] + \sin(hx_r) = 0 \qquad (6)$$

For getting a comparison between η and η_{cA} see Fig.10.



.(brown color η:and violet color:η_{cA})Fig.10: Variations of η and η_{cA} in terms of η_c

Therefore the variations of x_l as a function of η_c are plotted in fig.11.Also Our numerical calculated of physical parameters listed in Table.1

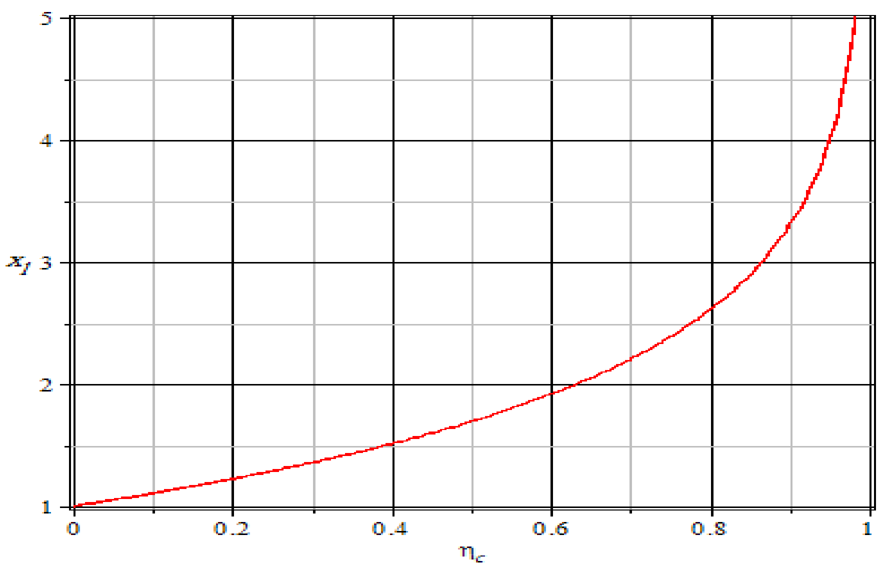


Fig.11: variations of x_l as a function of η_c

Table1:Our numerical calculated of physical parameters

$\frac{T_l}{T_r}$	η_c	η_T	η_c	η_S	η_c	η	η_c	η_{cA}	η_c	x_l	η_c
1	0	0	0	0	0	0.2	0	0	0	1	0

0.8	0.2	0.3	0.45	0.3	0.45	0.4	0.6	0.2	0.4	2	0.6
0.6	0.4	0.5	0.65	0.5	0.8	0.6	0.8	0.4	0.6	3	0.85
0.4	0.6	0.7	0.85	0.65	1.0	0.8	0.85	0.6	0.8	4	0.88
0	1	0.9	1			1	1	1	1	5	1

CONCLUSION

In conclusion, nanosystems with perfectly coupled fluxes, such as the quantum dot described here, are of great interest.This work presented a detailed thermodynamic analysis of electron transport through a single quantum dot connecting two leads at different temperatures and chemical potentials.The study of this model addresses several issues of timely interest: nanotechnology, the study of thermodynamic properties of small devices that are pronetofluctuations, the question of universality for thermodynamic properties away from equilibrium, the role of quantum features in this respect, and the promise of thermoelectricity generated by nanodevices.

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