Quantum bounds for power production, efficiency and thermal currents in thermoelectric nanostructures

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June 15, 2022

Abstract

The wave-like nature of electrons leads to the existence of upper bounds on the thermoelectric response of nanostructured devices [R. S. Whitney, Phys. Rev. Lett. 112, 130601 (2014); Phys. Rev. B 91, 115425 (2015)]. This fundamental result, not present in classical thermodynamics, was demonstrated exploiting a two-terminal device modelled by non-linear scattering theory. In the present paper, we consider non-linear quantum transport through the same type of device working both as thermal machine and as refrigerator. For both operations, starting from charge and heat current expressions, we provide analytic quantum bounds for power exchanged, thermal currents and device efficiencies. For this purpose, we adopt a thermoelectric system with a transmission function that corresponds to the quantum bound conditions, and show that we can recover the result with an alternative simple and transparent procedure.

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1 Introduction

Nanoscale thermoelectric (TE) engines for both power production and refrigeration have attracted great interest since the papers of Hicks and Dresselhaus [1–3] and of Mahan and Sofo [4], who evidenced the effect of reduced dimensionality on the electronic density of states to increase the TE efficiency. In linear regime conditions, i.e., for low temperature gradients and small applied voltage biases, the thermoelectric performance is represented by the dimensionless figure of merit [5] \( ZT = \sigma S^2 T / (\kappa_{el} + \kappa_{ph}) \), where \( \sigma \) is the electronic conductance, \( S \) the Seebeck coefficient, \( T \) the absolute temperature, and \( \kappa_{el} \) (\( \kappa_{ph} \)) the electronic (phonon) thermal conductance. Attempts to reach high values of \( ZT \) modifying the physical parameters entering in its definition by device design and appropriate choice of materials have shown limits due to their often competing behavior as function of temperature [6–15]. In fact, for nanostructures the non linear response regime is of primary interest because at the nanometer scale temperature and bias gradients may become very large. Description of thermoelectric phenomena at the nanoscale as in the case of quantum wells [16], quantum dots [17,18], nanowires [19], molecular junctions [20] or superlattices [21] deserves to consider fundamental aspects connected with quantum effects, thermodynamics and scale of electron thermalization [22–27]. Moreover, quantum transport formalism provides an appropriate microscopic description of charges and heat flows [28–30]. In particular, for non-interacting systems, calculations of thermoelectric functions also in multiterminal cases and in the
presence of magnetic fields \cite{31,32} can be done by means of the Landauer-Büttiker approach, which provides expressions for electron and heat currents in terms of transmission properties and contains the microscopic physics of the system. In the case many-body effects are important, the most appropriate approach is based on the Keldysh formalism \cite{28–30,33–38}.

In the present paper, we study a two-terminal device made of two reservoirs (left and right) at different temperatures and chemical potentials, \((T_L, \mu_L)\) and \((T_R, \mu_R)\), and connected to a central scattering region by perfect leads, see Fig. 1. We suppose that the device is in quantum coherent conditions, with no electron-phonon and electron-electron interactions. In the above quantum coherent regime, the Büttiker-Landauer scattering theory \cite{23,39,40} is used for the description of heat currents and electrical currents. This theory is valid for linear as well for non-linear regimes. Transport is described by the transmission function \(T(E)\) of the scattering region.

A further important aspect connected with the quantum nature of electrons has been highlighted by Whitney \cite{41,42} and addressed in what follows. The story goes back to the work of Bekenstein \cite{43} on the relation between information flow and energy flow rates, and the study of Lebedev and Levitin \cite{44}(1966) concerning the transmission of an electromagnetic field in one dimension and a single-channel communication system. In a successive work by means of information theory analogy, Pendry \cite{45}(1983) found a fundamental upper bound on the heat flow through a quantum system between a left reservoir at temperature \(T\) and a right reservoir at \(T=0\): 

\[
I_Q^{(Pendry)} \equiv (k_B T)^2 N \pi^2 / 6 \hbar,
\]

where \(k_B\) is the Boltzmann constant, \(N\) is the number of channels in the cross section through which current flows, and \(\hbar\) is the Planck constant.

Based on this result, for quantum thermoelectrics described by Landauer scattering theory, Whitney extended the Pendry's result by considering the heat flow through a scattering system between two reservoirs at different temperatures and at the same chemical potential. He found a quantum bound on the power output and then by an optimization process of the transmission function he obtained an upper bound for the efficiency at given power output for heat engines and for refrigerators.

The motivation of the present paper is to show that these results can be obtained with an alternative mathematical procedure starting from the expression of charge and heat currents. This sheds further light and clarification on the physical interpretation of quantum bounds in thermoelectric phenomena.

In Sec. 2, we provide basic expressions for thermoelectric transport through a two-terminal mesoscopic electronic system. These expressions are useful for the determination of the existence of quantum bounds in currents, exchanged power and machine efficiencies, and for their ana-

![Figure 1: Schematic representation of the scattering region S connected to two reservoirs. We consider positive the direction for the currents from the left to right.](image-url)
lytic evaluation. Section 3 and Sec. 4 present the explicit expressions for the above mentioned quantities. From them, it is easy to individuate the presence of upper values (quantum bounds) in thermoelectric transport. Sec. 5 and Sec. 6 address the same above problems in the case of very low power exchanged by thermal machines and refrigerators, respectively. Finally, Sec. 7 concludes.

2 Model and basic expressions for thermoelectric transport in nanoscale structures

In this section, we consider transport through a two-terminal mesoscopic electronic system coupled to two reservoirs, characterized by \( N \) transmitting channels, with total transmission function \( T(E) \leq N \). Without loss of generality, we assume that the temperature of the left reservoir \( T_L \) is higher than that of the right reservoir \( T_R \). We examine in detail the case \( \mu_L < \mu_R \). The opposite case \( \mu_L > \mu_R \) could be envisaged, with appropriate modifications, from the discussion here presented.

The left or the right thermal currents \( I^{(L)}_Q \) and \( I^{(R)}_Q \), and the output or input power \( P \), related to transport of electrons across the mesoscopic device are given by the Landauer expressions valid for linear and non-liner regimes \([39,46–48]\)

\[
I^{(L,R)}_Q = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE (E - \mu_{L,R}) T(E) \left[f_L(E) - f_R(E)\right] \tag{1a}
\]

\[
P = I^{(L)}_Q - I^{(R)}_Q = \frac{1}{\hbar} \left(\mu_R - \mu_L\right) \int_{-\infty}^{+\infty} dE T(E) \left[f_L(E) - f_R(E)\right] , \tag{1b}
\]

where \( f_{L,R}(E) = 1/[e^{(E-\mu_{L,R})/k_B T_{L,R}} + 1] \) are the Fermi-Dirac distribution functions in the two leads. The applied bias potential \( \Delta V = V_L - V_R \) and the chemical potentials difference \( \Delta \mu = \mu_L - \mu_R \) are related by \((-e)\Delta V = \Delta \mu\). The device operates as thermal machine, i.e, in the power production regime \( P = P_{\text{out}} > 0 \), when the heat is extracted from the hot reservoir and released to the cold one, while part of the thermal energy can be converted into usable power. We have thus the conditions

\[
I^{(L)}_Q > I^{(R)}_Q > 0 . \tag{2}
\]

The efficiency of the device in this mode is defined as the ratio of the usable power to the heat extracted from the hot reservoir

\[
\eta^{(tm)} = \frac{P_{\text{out}}}{I^{(L)}_Q} = \frac{I^{(L)}_Q - I^{(R)}_Q}{I^{(L)}_Q} \leq \eta^{(tm)}_c . \tag{3}
\]

As a consequence, the efficiency of the thermal machine cannot exceed the Carnot efficiency \( \eta^{(tm)}_c \equiv (T_L - T_R)/T_L \). The device operates as a refrigerator if heat is extracted from the cold reservoir and released into the hot reservoir, with the absorption of external energy converted into wasted heat. In this case, left thermal current, right thermal current and absorbed power (\( P = P_{\text{in}} \)) are all negative quantities:

\[
I^{(L)}_Q < I^{(R)}_Q < 0 , \tag{4}
\]
and the efficiency (coefficient of performance) of the refrigerator is given by

$$
\eta^{(refr)} = \frac{I^{(R)}_Q}{P_{in}} = \frac{I^{(R)}_Q}{I^{(L)}_Q - I^{(R)}_Q} \leq \eta^{(refr)}_c.
$$

As a consequence, the upper thermodynamic bound of the refrigeration efficiency cannot exceed the performance of the Carnot refrigerator \( \eta^{(refr)}_c \equiv \frac{T_R}{T_L - T_R} \).

From the transport Eqs. (1), it is apparent the basic role played by \( T(E) \) and by the difference of the Fermi functions of the left and right leads electrodes \( f_{LR}(E) \equiv f_L(E) - f_R(E) \). We notice that

$$
f_{LR}(E) > 0 \quad \text{if} \quad E > \frac{\mu_R T_L - \mu_L T_R}{T_L - T_R} \equiv \epsilon_0,
$$

where the energy \( \epsilon_0 \) separates the region of positive values of \( f_{LR}(E) \) from the region of negative values. The position of \( \epsilon_0 \) with respect to the two chemical potentials can be easily established as

$$
\epsilon_0 - \mu_{L,R} = \frac{T_{L,R}}{T_L - T_R}(\mu_R - \mu_L) > 0.
$$

Thus \( \epsilon_0 \) is at the right of the chemical potentials of the two reservoirs, as seen in Fig. 2.

From Eq. (7), we have

$$
\frac{\epsilon_0 - \mu_L}{k_B T_L} = \frac{\epsilon_0 - \mu_R}{k_B T_R} = \frac{\mu_R - \mu_L}{k_B(T_L - T_R)} \equiv x_0,
$$

where, as shown below, the quantity \( x_0 \) is important in the definition of quantum bounds for currents and exchanged power.

It is worth noticing that at the energy \( \epsilon_0 \) the occupation of states in the two electron reservoirs is the same and the two reservoirs can exchange electrons reversibly. As evident from Eqs. (1), for \( E = \epsilon_0 \) the exchanged power \( P \) becomes 0 and the thermal machine efficiency reaches the Carnot limit [49,50]:

$$
\eta^{(tm)} = P/(I^{(L)}_Q) = (\mu_R - \mu_L)/(\epsilon_0 - \mu_L) = 1 - T_R/T_L = \eta^{(tm)}_C.
$$

This coincides with the results of Mahan and Sofo for a delta-like shape transmission function filtering at the energy \( \epsilon_0 \) [4,51] and corresponds to reversible transport with zero entropy production and zero output power. Similar considerations can be done for the coefficient of performance in the refrigerator machine.

A further result of Whitney is the proof that the optimal efficiency of a thermal machine at a given power output is obtained when the transmission function has a square shape, which allows transmission of electrons only in a chosen energy range, the width of the square being determined by the maximum possible efficiency for a given power output [42,52].

### 3 Quantum transport through ideal thermal machines

#### 3.1 Quantum bounds for power generation

Consider a system in the power generation regime \( P > 0 \). The expression of the output power is given in Eq. (1b), whose maximal value is obtained restricting the integral to the positive region
Figure 2: (a) Representation on the energy axis of the functions \( (E - \mu_L) f_{LR}(E) \) (pointed line), \( (E - \mu_R) f_{LR}(E) \) (dashed line), and \( (\mu_R - \mu_L) f_{LR}(E) \) (solid line) which enter in the definition of the thermal currents, \( I^{(L)}_Q \) and \( I^{(R)}_Q \), and power \( \mathcal{P} \) respectively (see Eq. (1a) and Eq. (1b)), in the case \( T_L > T_R \) and \( \mu_L < \mu_R \). (b) Optimal (box-like shape) transmission function for the ideal refrigerator. It is different from zero, and equal to the number of transmission channels \( N \), only in the region \( \mu_R \leq E \leq \epsilon_0 \) where both \( I^{(L)}_Q \) and \( I^{(R)}_Q \) are negative. (c) Optimal (step-like shape) transmission function for the ideal thermal machine. It is different from zero, and equal to the number of transmission channels \( N \), only when \( E \geq \epsilon_0 \), where both \( I^{(L)}_Q \) and \( I^{(R)}_Q \) are positive. Without loss of generality, for this figure we have chosen \( T_L = 600 \) K, \( T_R = 300 \) K, \( \mu_L = 0 \) eV, and \( \mu_R = 0.025 \) eV.

of \( f_{LR}(E) \), see Fig. 2, and assuming the value of \( N \) for the total “optimal” transmission function in the whole domain \([\epsilon_0, \infty)\), i.e., a step-like shape for the transmission function of the ideal power generator. For this device the output power is given by the expression

\[
\mathcal{P}_{out} = \frac{N}{\hbar} (\mu_R - \mu_L) \int_{\epsilon_0}^{+\infty} dE f_{LR}(E) = \frac{N}{\hbar} k_B^2 (T_L - T_R)^2 \xi_0 \ln(1 + e^{-\xi_0}),
\]

(10)

where we exploited the definite integral \( \int_{\epsilon_0}^{+\infty} f(E) dE = k_B T \ln\left[ 1 + e^{-(E_0 - \mu)/k_B T}\right] \). We have now to optimize Eq. (10) when the chemical potentials of the leads are changed, at fixed temperatures \( T_L \) and \( T_R \), which means, in essence, to maximize the function \( F(x_0) = x_0 \ln(1 + e^{-x_0}) \). With numerical methods we find \( dF(x_0)/dx_0 = 0 \) for \( \bar{x}_0 = 1.146 \), where

\[
F(\bar{x}_0) = \bar{x}_0 \ln(1 + e^{-x_0}) \approx 0.316.
\]

(11)
In summary, the quantum bound for power production reads
\[
P_{\text{out}}^{(QB)} = C_0 \frac{N}{R} k_B^2 (T_L - T_R)^2 \quad \text{with} \quad C_0 \equiv 0.316 ,
\]
in complete agreement with Eq.(43) and Eq.(44) of ref. [42].

### 3.2 Quantum bounds for left thermal currents

The general expression of the left thermal current is given by Eq. (1a). Its value for a device in the *ideal power generation regime* is obtained restricting the integral to the positive region of \( f_{LR}(E) \), and assuming, as before, the value of \( N \) for the total transmission function in the whole domain \( [\epsilon_0, \infty] \). One has
\[
I_{LQ}^{(L)} = \frac{N}{h} \int_{\epsilon_0}^{+\infty} dE (E - \mu_L) f_{LR}(E) . \tag{13}
\]
This integral is evaluated analytically using the elementary properties of the poly-logarithm functions of order one, \( \text{Li}_1(z) \), and of order two, \( \text{Li}_2(z) \), (see App. A) Eq. (13) for \( I_{LQ}^{(L)} \) finally becomes (see App. B)
\[
I_{LQ}^{(L)} = \frac{N}{h} k_B^2 T_L (T_L - T_R) x_0 \ln(1 + e^{-x_0}) - \frac{N}{h} k_B^2 (T_L^2 - T_R^2) \text{Li}_2(-e^{-x_0}) . \tag{14}
\]
The thermal current depends on the difference of the chemical potentials, on the difference of the temperatures, on the left current and on the average temperature. In the particular case \( T_L = T_R \), the value of \( x_0 \) approaches \( \infty \) and no thermal current flows through the device.

To establish the quantum bound of the left thermal current with an eye to Eq. (14), we have to maximize the function
\[
G(x_0) = T_L x_0 \ln(1 + e^{-x_0}) - (T_L + T_R) \text{Li}_2(-e^{-x_0}) . \tag{15}
\]
The derivative of the above function, with the help of (56) becomes
\[
dG(x_0)/dx_0 = -T_L x_0/(e^{x_0} + 1) - T_R \ln(1 + e^{-x_0}) < 0 . \tag{16}
\]
Since \( x_0 \) is limited to values greater or equal to zero, we argue that the maximum value of the function \( G(x_0) \) occurs for \( x_0 = 0 \). Replacing this value into Eq. (14), we obtain that the maximum value of the left thermal current generated by a device in the power generation regime presents the quantum bound
\[
I_{LQ}^{(L)(QB)} = \frac{N \pi^2}{12} \frac{k_B^2}{h} (T_L^2 - T_R^2) , \tag{17}
\]
where we have used \( \text{Li}_2(-1) = -\pi^2/12 \).

### 3.3 Quantum bounds for right thermal currents

The maximal value of the right thermal current of Eq. (1a) in the power generation regime, can be evaluated following step-by-step the procedure applied to the expression of the left thermal current of Eq. (13). For the right thermal current, we obtain the expression
\[
I_{Q}^{(R)(QB)} = \frac{N}{h} k_B^2 T_\tilde{R}(T_L - T_R) x_0 \ln(1 + e^{-x_0}) - \frac{N}{h} k_B^2 (T_L^2 - T_R^2) \text{Li}_2(-e^{-x_0}) . \tag{18}
\]
By setting $\mu_R = \mu_L$, i.e., $x_0 = 0$ in Eq. (18), we obtain that the maximal value of the right thermal current generated by a device in the power generation regime presents the quantum bound

$$I_Q^{(R)(QB)} = \frac{N \pi^2}{12} \frac{k_B^2}{h} (T_L^2 - T_R^2).$$

This quantum bound is of course the same as the quantum bound for the left thermal current, in fact, when the two chemical potentials are equal, also the two thermal currents must be equal.

### 3.4 Quantum bound for efficiency in a power generator

The expression of the efficiency of the thermal machine reads

$$\eta^{(tm)} = \frac{\mathcal{P}_{\text{out}}}{I_Q^{(L)}} = \frac{(T_L - T_R)x_0 \ln(1 + e^{-x_0})}{T_L x_0 \ln(1 + e^{-x_0}) - (T_L + T_R) \text{Li}_2(-e^{-x_0})} = \frac{\eta_C^{(tm)}}{1 - \frac{(T_L + T_R)}{T_L x_0 \ln(1 + e^{-x_0})} \text{Li}_2(-e^{-x_0})}.$$  

(20)

![Figure 3: Behavior of the function $\frac{\text{Li}_2(-e^{-x_0})}{x_0 \ln(1 + e^{-x_0})}$.](image)

We can see that when $\mu_L \approx \mu_R$ no efficient thermal machine is possible. On the contrary the maximal efficiency of Eq. (20) is obtained when $x_0 \to \infty$, see Fig. 3. The maximal efficiency equals the thermodynamic bound of the Carnot machine, while the production of power is vanishingly small.

### 4 Quantum transport through ideal refrigerators

#### 4.1 Absence of quantum bounds for the absorbed power

In this section, we study transport through a device perfectly transparent in the refrigeration domain and perfectly opaque elsewhere. For a device operating in the ideal refrigeration mode, i.e., with left thermal current, right thermal current and absorbed power all negative quantities,
we have to restrict the integral defining their expressions to the negative region of $f_{LR}(E)$ in the domain $[\mu_R, \epsilon_0]$, and assuming the “optimal” value of $N$ for the transmission function there, see Fig. 2, i.e., for the transmission function it is assumed a box-like shape of width $(\epsilon_0 - \mu_R)$: $\mathcal{T}(E) = N$ for $\mu_R < E < \epsilon_0$ and $\mathcal{T}(E) = 0$ elsewhere. In this case, the right thermal current is maximal. For the described nanostructure device in the refrigeration regime ($\mathcal{P} < 0$) the expression of the absorbed (input) power reads

$$\mathcal{P}_{in} = \frac{N}{\hbar} (\mu_R - \mu_L) \int_{\mu_R}^{\epsilon_0} dE f_{LR}(E) . \quad (21)$$

The above integral can be performed analytically (see App. B) and gives

$$\mathcal{P}_{in} = \frac{N (\mu_R - \mu_L)}{\hbar} \left[ -k_B T_L \ln(1+e^{-x_0}) + k_B T_L \ln(1+e^{-x_1}) + k_B T_R \ln(1+e^{-x_0}) - k_B T_R \ln 2 \right] , \quad (22)$$

where $x_1 \equiv (\mu_R - \mu_L)/(k_B T_L)$. In particular, we remark

$$\mathcal{P}_{in} = -\frac{N (\mu_R - \mu_L)}{\hbar} k_B T_R \ln 2 + \ldots \quad \text{for} \quad \mu_R - \mu_L \to +\infty . \quad (23)$$

For arbitrary large difference of the chemical potentials, it is evident that no bound occurs for the absorbed power. This is different from the situation of thermal machine, where an upper bound occurs for power generation.

### 4.2 Left thermal current: absence of quantum bound

The left thermal current in the ideal refrigerator is

$$I_Q^{(L)} = \frac{N}{\hbar} \int_{\mu_R}^{\epsilon_0} dE (E - \mu_L) f_{LR}(E) . \quad (24)$$

Details of the manipulation of the above equation are reported in the in App. B. The final expression of Eq. (24) is

$$I_Q^{(L)} = \frac{N}{\hbar} \left[ -k_B T_R (\mu_R - \mu_L) \ln 2 + k_B^2 T_L^2 x_1 \ln(1+e^{-x_1}) + k_B^2 (T_L^2 - T_R^2) \mathrm{Li}_2(-e^{-x_0}) 
- k_B^2 T_L T_R x_0 \ln(1+e^{-x_0}) - k_B^2 T_L^2 \mathrm{Li}_2(-e^{-x_1}) + k_B^2 T_R^2 \mathrm{Li}_2(-1) \right] . \quad (25)$$

In particular, remembering the definitions of $x_0$ and $x_1$, we find the leading terms

$$I_Q^{(L)} = -\frac{N}{\hbar} k_B T_R (\mu_R - \mu_L) \ln 2 + \frac{N}{\hbar} k_B^2 T_L^2 \mathrm{Li}_2(-1) + \ldots \quad \text{for} \quad \mu_R - \mu_L \to +\infty . \quad (26)$$

For arbitrary large difference of the chemical potentials, it is evident that no bound occurs for the intensity of the left thermal current. This is different from the situation of thermal machine, where an upper bound occurs for the left thermal current.

### 4.3 Quantum bound for the right thermal current

By proceeding as above, the right thermal current is

$$I_Q^{(R)} = \frac{N}{\hbar} \int_{\mu_R}^{\epsilon_0} dE (E - \mu_R) f_{LR}(E) . \quad (27)$$
After some algebra, we obtain the expression

\[
I^{(R)}_Q = \frac{N}{\hbar} \left[ k_B^2 (T_L^2 - T_R^2) L_2 (-e^{-x_0}) - k_B^2 T_R (T_L - T_R)x_0 \ln(1 + e^{-x_0})
\right.
\]
\[
- k_B^2 T_L^2 L_2 (-e^{-x_1}) + k_B^2 T_R^2 L_2 (-1) \right].
\]  
(28)

We have that

\[
I^{(R)}_Q = \frac{N}{\hbar} k_B^2 T^2 L_2 (-1) + \ldots \text{ for } \mu_R - \mu_L \rightarrow +\infty .
\]  
(29)

In conclusion, a quantum bound exists for the negative right thermal current

\[
\left| I^{(R)}_Q \right| < \frac{N \pi^2 k_B^2}{12} T^2 L_2 \equiv I^{(R)(QB)}_Q.
\]  
(30)

The above result is in agreement with that reported in Eq.(58) of ref. [42], considering that we define

\[
I^{(R)(QB)}_Q = \frac{1}{2} I^{(Pendry)}_Q.
\]  
(31)

5 Quantum transport in a thermal machine at low-power output.

We consider quantum transport through a device in the low-power generation regime, i.e., in the case \( \mathcal{P} \approx 0^+ \). The ideal low-power generation regime is obtained restricting the integral in Eq. (1b) to the positive region of \( f_{L,R}(E) \), and assuming the value of \( N \) for the transmission function in the small domain \([\epsilon_0, \epsilon_0 + \Delta]\) (i.e., a box-car shape of width \( \Delta \), see Fig. 1). Namely, we assume \( T(E) = N \) for \( \epsilon_0 < E < \epsilon_0 + \Delta \), with \( \Delta \rightarrow 0^+ \), and \( T(E) = 0 \) otherwise. The low-power output becomes

\[
\mathcal{P}_{\text{out}} = \frac{N}{\hbar} (\mu_R - \mu_L) \int_{\epsilon_0}^{\epsilon_0 + \Delta} dE f_{L,R}(E).
\]  
(32)

Proceeding as in App. C, one can show that the final result is

\[
\mathcal{P}_{\text{out}} = \frac{N}{\hbar} (\mu_R - \mu_L) \left[ \frac{\Delta^2 (T_L - T_R)}{2k_B T_L T_R} \psi'(x_0) + \frac{\Delta^3 (T_L^2 - T_R^2)}{6k_B^2 T_L^2 T_R^2} \psi''(x_0) + O(\Delta^4) \right],
\]  
(33)

where \( \psi(x) = -1/(e^x + 1) \).

5.1 Left thermal current in low-power ideal generators

Following App. C, the left thermal current is

\[
I^{(L)}_Q = \frac{N}{\hbar} \int_{\epsilon_0}^{\epsilon_0 + \Delta} dE (E - \mu_L) f_{L,R}(E)
\]
\[
= \frac{N}{\hbar} (\mu_R - \mu_L) \frac{T_L}{T_L - T_R} \left[ \frac{\Delta^2 (T_L - T_R)}{2k_B T_L T_R} + \psi'(x_0) + \frac{\Delta^3 (T_L^2 - T_R^2)}{6k_B^2 T_L^2 T_R^2} \psi''(x_0) \right]
\]
\[
+ \frac{N}{\hbar} \frac{\Delta^3 (T_L - T_R)}{3k_B T_L T_R} \psi'(x_0) + O(\Delta^4).
\]  
(34)
Using Eq. (33), we obtain the more effective form

$$I_Q^{(L)} = \frac{T_L}{T_L - T_R} \mathcal{P}_{\text{out}} + \frac{N}{\hbar} \frac{\Delta^3(T_L - T_R)}{3k_B T_L T_R} \psi'(x_0) + O(\Delta^4),$$

(35)

which exactly coincides with Eq.(47) of ref. [42].

### 5.2 Efficiency of low-power thermal machines

We can divide both members of Eq. (35) by $I_Q^{(L)}$ and obtain

$$\eta^{(\text{tm})} = \frac{\mathcal{P}_{\text{out}}}{I_Q^{(L)}} = \frac{T_L - T_R}{T_L} \left[ 1 - \frac{N}{\hbar} \frac{\Delta^3(T_L - T_R)}{3k_B T_L T_R} \psi'(x_0) \right].$$

(36)

Linear corrections in the $\Delta$ parameter can be obtained expressing $I_Q^{(L)}$ to quadratic terms in the $\Delta$ parameter from Eq. (34). Eventually, we find

$$\eta^{(\text{tm})} = \eta^{(\text{tm})}_{c} \left[ 1 - \frac{2}{3} \frac{\Delta}{k_B T_L x_0} + O(\Delta^2) \right]$$

(37)

thus recovering Eq.(49) of ref. [42].

### 5.3 Efficiency of low-power thermal machines at fixed power output

The expression for the power production of the low-power thermal machine is given by Eq. (33). At the lowest (quadratic) order in $\Delta$, the usable power reads

$$\mathcal{P}_{\text{out}} = \frac{N}{\hbar} x_0 \frac{\Delta^2(T_L - T_R)^2}{2T_L T_R} \psi'(x_0).$$

(38)

It is convenient to normalize the output power with the quantum bound obtained in Eq. (12) and we have

$$\frac{\mathcal{P}_{\text{out}}}{\mathcal{P}_{\text{out}}^{(\text{QB})}} = \frac{1}{C_0} \frac{\Delta^2}{2k_B T_L T_R} x_0 \psi'(x_0).$$

(39)

Combining Eq. (37) with the above equation we obtain

$$\eta^{(\text{tm})} = \eta^{(\text{tm})}_{c} \left[ 1 - \frac{2}{3} \sqrt{2C_0} \frac{T_R \mathcal{P}_{\text{out}}}{T_L \mathcal{P}_{\text{out}}^{(\text{QB})}} \frac{1}{\sqrt{x_0^3 \psi'(x_0)}} \right].$$

(40)

The last step to be performed is the maximization of the above expression.

### 5.4 Optimization of the efficiency of low-power thermal machine at fixed power output

Optimization of the efficiency at given temperatures requires the maximization of the function $H(x_0) = +x_0^3 \psi'(x_0)$, which appears in the denominator of Eq. (40). With standard methods, we find

$$\bar{x}_0 = 3.24 \quad \text{and} \quad H(\bar{x}_0) = 1.234.$$
Considering that according to Eq. (12) \( C_0 = 0.316 \), we have for the coefficient \( (2/3)\sqrt{2C_0/H(x_0)} \) the value 0.477. Finally, we obtain
\[
\eta^{(tm)} = \eta_c^{(tm)} \left[ 1 - 0.477 \sqrt{\frac{P_{\text{out}}}{P_{\text{out}}} - \frac{P_{\text{out}}}{P_{\text{out}}}} \right].
\] (42)

This relation coincides with Eq.(51) of ref. [42].

6 Quantum transport in a refrigerator at low-cooling regime

The ideal low-power refrigerator \( (P \approx 0^-) \) is obtained restricting the integral to the negative region of \( f_{LR}(E) \), and assuming the value of \( N \) for the transmission function in the small domain \( [\epsilon_0 - \Delta, \epsilon_0] \), see Fig. 2, i.e., we assume \( T(E) = N \) for \( \epsilon_0 - \Delta < E < \epsilon_0 \) and \( T(E) = 0 \) otherwise, with \( \Delta \to 0^+ \). For the low-cooling refrigerator, the absorbed power is then
\[
P_{\text{in}} = \frac{N}{h}(\mu_R - \mu_L) \int_{\epsilon_0 - \Delta}^{\epsilon_0} dE f_{LR}(E). \] (43)

With an eye to App. C, the power absorption becomes
\[
P_{\text{in}} = \frac{N}{h}(\mu_R - \mu_L) \left[ -\frac{\Delta^2(T_L - T_R)}{2k_B T_L T_R} \psi'(x_0) + \frac{\Delta^3(T_L^2 - T_R^2)}{6k_B^2 T_L^2 T_R^2} \psi''(x_0) \right] + O(\Delta^4). \] (44)

6.1 Right thermal current for an ideal refrigerator in the low-cooling regime

In the present conditions, the right thermal current is
\[
I_Q^{(R)} = \frac{N}{h} \int_{\epsilon_0 - \Delta}^{\epsilon_0} dE (E - \mu_R)f_{LR}(E)
\]
\[
= \frac{N}{h}(\mu_R - \mu_L) \left[ -\frac{\Delta^2(T_L - T_R)}{2k_B T_L T_R} \psi'(x_0) + \frac{\Delta^3(T_L^2 - T_R^2)}{6k_B^2 T_L^2 T_R^2} \psi''(x_0) \right] + \frac{N \Delta^3(T_L - T_R)}{h 3k_B T_L T_R} \psi'(x_0) + O(\Delta^4). \] (45)

Exploiting Eq. (44) for \( P_{\text{in}} \), equation Eq. (45) can be cast in the more effective form
\[
I_Q^{(R)} = \frac{T_R}{T_L - T_R} P_{\text{in}} + \frac{N \Delta^3(T_L - T_R)}{h 3k_B T_L T_R} \psi'(x_0). \] (46)

This equation coincides with Eq.(59) of ref. [42], where \( T_R \) and \( T_L \) are exchanged.

6.2 Efficiency of an ideal refrigerator in the low-cooling regime

The general expression for the efficiency of the refrigerator machine reads
\[
\eta^{(\text{refr})} = \frac{I_Q^{(R)}}{P_{\text{in}}} = \frac{T_R}{T_L - T_R} \left[ 1 + \frac{N \Delta^3(T_L - T_R)^2}{h 3k_B T_L T_R^2} \psi'(x_0) \frac{1}{P_{\text{in}}} \right]. \] (47)
Correction linear in the $\Delta$ parameter can be obtained expressing $P_{in}$ to quadratic terms in the $\Delta$ parameter. From Eq. (44) it holds

$$P_{in} = -\frac{N}{h} (\mu_R - \mu_L) \frac{\Delta^2 (T_L - T_R)}{2k_B T_L T_R} \psi'(x_0) + O(\Delta^3)$$

Inserting Eq. (48) into Eq. (47) gives

$$\eta^{(refr)} = \eta^{(refr)}_c \left[ 1 - \frac{2}{3} \frac{\Delta}{k_B T_R x_0} + O(\Delta^2) \right],$$

which corresponds to Eq.(61) of ref. [42].

6.3 Efficiency of the low-cooling refrigerator at fixed power input

The expression for the right thermal current of the low-power refrigeration machine is given by Eq. (45). At the lowest (quadratic) order in $\Delta$, the right thermal current reads

$$I_Q^{(R)} = -\frac{N}{h} x_0 \frac{\Delta^2 (T_L - T_R)}{2T_L} \psi'(x_0).$$

As done in Eq.(20) of ref. [42], we normalize the right thermal current as

$$\frac{I_Q^{(R)}}{I_Q^{(Pendry)}} = \frac{1}{2C_1} \frac{\Delta^2 (T_L - T_R)}{k_B T_L T_R^2} x_0 \psi'(x_0) \quad \text{with} \quad C_1 = \frac{\pi^2}{6}.$$ (51)

The expression of $\Delta$ from the above equation can be inserted in Eq. (47) and one obtains

$$\eta^{(refr)} = \eta^{(refr)}_c \left[ 1 - \frac{2}{3} \sqrt{\frac{T_L}{T_L - T_R}} \frac{I_Q^{(R)}}{I_Q^{(Pendry)}} \frac{1}{\sqrt{x_0^3 \psi'(x_0)}} \right].$$ (52)

The last step to be performed is the maximization of the above expression.

6.4 Optimization of the efficiency of the low-power refrigerator at fixed power absorption

Optimization of the efficiency at fixed temperatures requires in essence the maximization of the function $H(x_0) = +x_0^3 \psi'(x_0)$, with $H(x_0) > 0$. This function appears in the denominator of Eq. (52). This can be done repeating step by step the same process used for the case of the low-power thermal machine at fixed power output in Section 5. In particular, by exploiting the value of the coefficient $C_1 = 1.645$ we obtain $(2/3) \sqrt{2C_1} / H(x_0) = 1.088$. Finally, the maximal value of Eq. (47) is

$$\eta^{(refr)} = \eta^{(refr)}_c \left[ 1 - 1.088 \sqrt{\frac{T_L}{T_L - T_R}} \frac{I_Q^{(R)}}{I_Q^{(Pendry)}} \right],$$ (53)

which recovers exactly Eq.(63) of ref. [42].
**Ideal thermal machine**

\[ T(E) := \begin{cases} N, & E \geq \epsilon_0 \\ 0, & E < \epsilon_0 \end{cases} \]

**Ideal refrigerator**

\[ T(E) := \begin{cases} N, & \mu_R \leq E \leq \epsilon_0 \\ 0, & \text{Otherwise} \end{cases} \]

| \( P^{(QB)} \) | \( P_{out}^{(QB)} = C_0 \frac{N}{R} k_B^2 (T_L - T_R)^2 \) | Absence of bound for \( P_{in} \) |
|---|---|---|

| \( I_Q^{(L)(QB)} \) | \( \frac{N\pi^2 k_B^2}{12} \frac{k_B^2}{\hbar} (T_L^2 - T_R^2) \) | Absence of bound for \( I_Q^{(L)} \) |

| \( I_Q^{(R)(QB)} \) | \( \frac{N\pi^2 k_B^2}{12} \frac{k_B^2}{\hbar} (T_L^2 - T_R^2) \) | \( \frac{N\pi^2 k_B^2}{12} \frac{k_B^2}{\hbar} T_R^2 \) |

| \( \eta \) | \( \eta^{(tm)} \rightarrow \eta_C^{(tm)} \) | Absence of bound for \( \eta^{(refr)} \) |

Table 1: Transmission functions, quantum bounds and efficiency for the ideal thermal machine and for the ideal refrigerator.

### 7 Conclusions

We have presented a workable analytic procedure to demonstrate the presence of bounds in the thermoelectric response functions induced by the quantum nature of electrons. We have considered a two-terminal macroscopic device operating between two reservoirs at different temperatures and chemical potentials. The electronic transport in the device is modelled by the Landauer scattering theory and the electronic transmission function \( T(E) \) is assumed to be step-like shape or box-like shape, in the case of power generation machine or refrigerator machine, respectively, so to guarantee the condition of upper bound value of the thermoelectric parameters. The expressions obtained are summarized in tables 1 and 2. Our results show that the findings of ref. [42] can be obtained in a transparent way from the analytic evaluation of currents. Also in the case of vanishing width of the box-shaped transmission function, corresponding to low power output and low power absorption for thermal machines and refrigerators, respectively, we exactly recover expressions of ref. [42].
Low-power output ideal thermal machine

\[ T(E) := \begin{cases} N, & \epsilon_0 \leq E \leq \epsilon_0 + \Delta, \quad \Delta \to 0^+ \\ 0, & \text{Otherwise} \end{cases} \]

Refrigerator in the low-cooling regime

\[ T(E) := \begin{cases} N, & \epsilon_0 - \Delta \leq E \leq \epsilon_0, \quad \Delta \to 0^+ \\ 0, & \text{Otherwise} \end{cases} \]

\[ \eta^{(tm)} \sim \eta^{(rm)} C \left[ \sqrt{\frac{T_R}{T_L}} \frac{P_{\text{out}}}{P_{\text{out}}(QB)} \right] \]

\[ \eta^{(refr)} \sim \eta^{(refr)} C \left[ 1 - 1.088 \sqrt{\frac{T_L}{T_L - T_R}} \right] \frac{I_Q^{(R)}}{I_Q^{(R)(QB)}} \]

Table 2: Transmission functions and maximum efficiencies for the ideal thermal machine and the refrigerator in the low-power and low-cooling regimes, respectively.

Acknowledgments

G.M. acknowledges support from the University of Pisa under the “PRA - Progetti di Ricerca di Ateneo” (Institutional Research Grants) - Project No. PRA 2020-2021 92

A Polylogarithms basic properties

The polylogarithm function of order unit is defined in terms of the standard logarithm as [53]

\[ \text{Li}_1(z) \equiv -\ln(1 - z) = \sum_{n=1}^{\infty} \frac{z^n}{n} , \quad |z| < 1. \]

In general, one defines the polylog of order \( k \) as

\[ \text{Li}_k(z) \equiv \int_0^z \frac{\text{Li}_{k-1}(t)}{t} \, dt = \sum_{n=1}^{\infty} \frac{z^n}{n^k} \quad k = 2, 3, \ldots \]

where again the series expansion is valid in the \( |z| < 1 \) region. These functions inherit from the logarithm the branch point at \( z = 1 \) and the cut along the positive real axis \([1, +\infty)\). Considering \( z = -e^{-x} \) one obtains

\[ \frac{d}{dx} \text{Li}_m(-e^{-x}) = -\text{Li}_{m-1}(-e^{-x}) \quad m = 1, 2, \ldots \]

Notice in particular that

\[ \text{Li}_0(-e^{-x}) = -\frac{d}{dx} \text{Li}_1(-e^{-x}) = -\frac{1}{e^x + 1} . \]

The above functions are useful for calculating integrals related to the Fermi functions. In fact

\[ \int \frac{1}{e^x + 1} \, dx = -\int \text{Li}_0(-e^{-x}) \, dx = \text{Li}_1(-e^{-x}) = -\ln(1 + e^{-x}) \]
and integrating by parts
\[
\int \frac{x}{e^x+1} \, dx = \int x \frac{d}{dx} \ln(1 + e^{-x}) \, dx = x \ln(1 + e^{-x}) - \int \ln(1 + e^{-x}) \, dx
\]
\[
= -x \ln(1 + e^{-x}) + \text{Li}_2(-e^{-x}).
\]

Asymptotic behaviors [53] for \(x \to +\infty\) can be obtained easily as
\[
\text{Li}_1(-e^{-x}) = -e^{-x} + O(e^{-2x}) \quad \text{and} \quad \text{Li}_2(-e^{-x}) = -e^{-x} + O(e^{-2x}),
\]
moreover, for \(x \to -\infty\)
\[
\text{Li}_1(-e^{-x}) = x - e^x + O(e^{2x}) \quad \text{and} \quad \text{Li}_2(-e^{-x}) = -\frac{\pi^2}{6} - \frac{x^2}{2} + e^x + O(e^{2x}).
\]

### B Currents and power related integrals

Let us introduce two primitive functions involving the Fermi function
\[
g(E) \equiv \int \frac{1}{e^{\beta(E-\mu)} + 1} \, dE = \frac{1}{\beta} \text{Li}_1(-e^{-\beta(E-\mu)})
\]
and
\[
h(E) \equiv \int \frac{E}{e^{\beta(E-\mu)} + 1} \, dE = Eg(E) + \frac{1}{\beta^2} \text{Li}_2(-e^{-\beta(E-\mu)}),
\]
which follow from (58) and (59), respectively, and \(\beta = 1/k_B T\). Notice that both \(g(E)\) and \(h(E)\) are exponentially small when \(E \to +\infty\).

With the help of (62) and (63) we can quickly express the integrals reported in the main text. In fact
\[
\int f_{LR}(E) \, dE = g_L(E) - g_R(E)
\]
\[
\int (E-\mu)f_{LR}(E) \, dE = h_L - h_R - \mu(g_L - g_R)
\]
\[
= (E-\mu)(g_L(E) - g_R(E))
\]
\[
+ \beta_L^{-2} \text{Li}_2(-e^{-\beta_L(E-\mu_L)}) - \beta_R^{-2} \text{Li}_2(-e^{-\beta_R(E-\mu_R)}),
\]
where \(g_{L,R}(E)\) mean that \(g(E)\) is calculated in correspondence of \(T_{L,R}\) and \(\mu_{L,R}\). From application of expressions (64) we recover the results reported in the main text. For example, for the left current in the thermal machine mode we need to evaluate
\[
\int_{\epsilon_0}^{+\infty} (E-\mu_L)f_{LR}(E) \, dE = -(\epsilon_0 - \mu_L)(g_L(\epsilon_0) - g_R(\epsilon_0)) +
\]
\[
- \beta_L^{-2} \text{Li}_2(-e^{-\beta_L(\epsilon_0-\mu_L)}) + \beta_R^{-2} \text{Li}_2(-e^{-\beta_R(\epsilon_0-\mu_R)})
\]
\[
= k_B^2 T_L(T_L - T_R) x_0 \ln(1 + e^{-x_0}) - k_B^2 (T_L^2 - T_R^2) \text{Li}_2(-e^{-x_0}),
\]
where
we exploited the asymptotic expressions (60) and the definition of $e_0$ and $x_0$ given in the main text.

In the refrigerator mode the expressions are more involved because both integration limits are finite. For the left current we need

$$\int_{\mu_r}^{e_0} (E - \mu_L)f_{LR}(E) \, dE = (e_0 - \mu_L)(g_L(e_0) - g_R(e_0)) - (\mu_R - \mu_L)(g_L(\mu_R) - g_R(\mu_R)) + \beta_L^{-2}[\text{Li}_2(-e^{-x_0}) - \text{Li}_2(-e^{-x_1})] - \beta_R^{-2}[\text{Li}_2(-e^{-x_0}) - \text{Li}_2(-1)] .$$

After some algebra, one obtains

$$\int_{\mu_r}^{e_0} (E - \mu_L)f_{LR}(E) \, dE = k_B^2(T_L - T_R)x_0 \left[ -\ln(2) T_R + T_L \ln(1 + e^{-x_1}) - \ln(1 + e^{-x_0}) \right] + k_B^2(T_L^2 - T_R^2) \text{Li}_2(-e^{-x_0}) - k_B^2 T_L^2 \text{Li}_2(-e^{-x_1}) - \frac{\pi^2}{12} k_B^2 T_R^2 ,$$

as reported in the main text. The same procedure gives for the right current

$$\int_{\mu_r}^{e_0} (E - \mu_R)f_{LR}(E) \, dE = (e_0 - \mu_R)(g_L(e_0) - g_R(e_0)) + \beta_L^{-2}[\text{Li}_2(-e^{-x_0}) - \text{Li}_2(-e^{-x_1})] - \beta_R^{-2}[\text{Li}_2(-e^{-x_0}) - \text{Li}_2(-1)] + k_B^2(T_L^2 - T_R^2) \text{Li}_2(-e^{-x_0}) - k_B^2 T_L^2 \text{Li}_2(-e^{-x_1}) - \frac{\pi^2}{12} k_B^2 T_R^2 .$$

For the input power, the integral is

$$(\mu_R - \mu_L) \int_{\mu_r}^{e_0} f_{LR}(E) \, dE = (\mu_R - \mu_L)(g_{LR}(e_0) - g_{LR}(\mu_R)) = k_B(T_L - T_R)x_0 \left[ -\ln(2) T_R + (T_L - T_R) \ln(1 + e^{-x_0}) + T_L \ln(1 + e^{-x_1}) \right] .$$

C The low power regime

In this regime the integration limits are very close. This means that we can use the Taylor expansion of the $g$ and $h$ functions introduced in (62) and (63). The procedure is quite similar for all the needed integrals, so we present some details only for one case. For instance, for the power in the thermal machine mode we need

$$\int_{e_0}^{e_0 + \Delta} f_{LR}(E) \, dE = g_{LR}(e_0 + \Delta) - g_{LR}(\Delta) = g_{LR}^{\prime}(e_0) \Delta + g_{LR}^{\prime\prime}(e_0) \frac{\Delta^2}{2} + g_{LR}^{\prime\prime\prime}(e_0) \frac{\Delta^3}{6} + O(\Delta^4)$$

$$= f_{LR}(e_0) \Delta + f_{LR}^{\prime}(e_0) \frac{\Delta^2}{2} + f_{LR}^{\prime\prime}(e_0) \frac{\Delta^3}{6} + O(\Delta^4) .$$
Now using the fact that $f_{LR}(\varepsilon_0) = 0$ and the function $\psi(x) = -1/(e^x + 1)$ as defined in the main text, we find

$$f'_{LR}(\varepsilon_0) = (\beta_L - \beta_R) \frac{-e^{\varepsilon_0}}{(e^{\varepsilon_0} + 1)^2} = \frac{T_L - T_R}{k_B T_L T_R} \psi'(x_0)$$

(71)

$$f''_{LR}(\varepsilon_0) = (\beta_L^2 - \beta_R^2) \frac{e^{\varepsilon_0}(e^{\varepsilon_0} - 1)}{(e^{\varepsilon_0} + 1)^3} = \frac{T_L^2 - T_R^2}{k_B^2 T_L^2 T_R^2} \psi''(x_0)$$

(72)

and finally

$$\int_{\varepsilon_0}^{\varepsilon_0+\Delta} f_{LR}(E) \, dE = \frac{T_L - T_R}{2k_B T_L T_R} \psi'(x_0) \Delta^2 + \frac{T_L^2 - T_R^2}{6k_B^2 T_L^2 T_R^2} \psi''(x_0) \Delta^3 + O(\Delta^4)$$

(73)

as used in (33).

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