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Thermoelectric efficiency of critical quantum junctions

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We derive the efficiency at maximal power of a scale-invariant (critical) quantum junction in exact form. Both Fermi and Bose statistics are considered. We show that time-reversal invariance is spontaneously broken. For fermions we implement a new mechanism for efficiency enhancement above the Curzon-Ahlborn bound, based on a shift of the particle energy in each heat reservoir, proportional to its temperature. In this setting fermionic junctions can even reach at maximal power the Carnot efficiency. Bosonic junctions at maximal power turn out to be less efficient than fermionic ones.

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There is recently much interest in the study of thermoelectric phenomena in nanoscale devices and in particular, in nanoscale engines. The efficiency of such engines is a fascinating physical problem. As is well known, one relevant parameter for studying this problem is the efficiency $\eta(P_{\text{max}})$ at maximal power $P_{\text{max}}$. In the context of classical linear endoreversible thermodynamics (irreversible heat transfer) it has been shown \cite{1,2} that

$$\eta(P_{\text{max}}) \leq 1 - \sqrt{\frac{T_2}{T_1}} \equiv \eta_{\text{CA}},$$  \hspace{1cm} (1)

where $T_1 > T_2$ are the temperatures of the two reservoirs, needed for running the engine. The inequality (1) is known as Curzon-Ahlborn (CA) bound. In a series of recent papers \cite{3-7} it has been proposed that at the quantum level $\eta(P_{\text{max}})$ might be enhanced in principle above $\eta_{\text{CA}}$ by means of an explicit breaking of time-reversal symmetry. For this purpose, the authors of \cite{3-7} considered in the linear response regime a three-terminal setup with one probe terminal and a magnetic field, which breaks down time-reversal. A generalization of this idea to multi-terminal systems has also been studied \cite{8}.

In the present paper we investigate the efficiency of quantum Schrödinger junctions with both Fermi and Bose statistics. We demonstrate that when the interaction, driving the system away from equilibrium is scale invariant (critical), one can go beyond the linear response approximation and derive $\eta(P_{\text{max}})$ in exact form. Time reversal invariance is spontaneously broken, which provides in the quantum world an attractive alternative to the explicit breaking in \cite{3-7}. For fermions we propose and investigate a new mechanism for efficiency enhancement above $\eta_{\text{CA}}$, based on a shift of the energy in the heat reservoirs proportional to their temperature. With an appropriate shift, fermionic junctions can reach at maximal power even the Carnot efficiency $\eta_{\text{C}}$. Analogous behavior has been observed \cite{8} in the stochastic model of an isothermal engine. At maximal power the bosonic junctions are less efficient and do not attain $\eta_{\text{C}}/2$.

The system: The scheme of the junction, considered in this Letter, is shown in Fig. 1. The two thermal reservoirs at (inverse) temperature $\beta_i$ and chemical potential $\mu_i$ are connected with two semi-infinite leads through a point-like interaction characterized by a unitary scattering matrix $S$. The leads $L_i$ are modeled by two half-lines with local coordinates $\{x,\mu\} : x < 0, i = 1, 2$, $S$ being localized at $x = 0$. The system is away from equilibrium provided that $S$ has a non-vanishing transmission amplitudes and $\beta_1$ and/or $\mu_1$ differ from $\beta_2$ and/or $\mu_2$. The dynamics is fixed by the Schrödinger equation

$$i\hbar \partial_t + \frac{1}{2m} \partial_x^2 - \frac{a}{\beta_i} \psi(t, x, i) = 0,$$ \hspace{1cm} (2)

where $m$ is the mass and $a$ is a dimensionless real parameter. We show in what follows that the term $a/\beta_i$ (a temperature dependent potential), generating a shift in the dispersion relations

$$\omega_i(k) = \frac{k^2}{2m} + \frac{a}{\beta_i},$$ \hspace{1cm} (3)

of the particles in the two heat baths, affects $\eta(P_{\text{max}})$.

We adopt a field theory formulation. Accordingly, the Schrödinger field $\psi(t, x, i)$ with (Fermi) Bose statistics satisfies the standard equal-time canonical (anti)commutation relations. The interaction at the point $x = 0$ is fully codified in the boundary condition

$$\lim_{x \to 0^-} \sum_{j=1}^{2} [g(\mathbb{1} - U)_{ij} + i(\mathbb{1} + U)_{ij} \partial_x] \psi(t, x, j) = 0,$$ \hspace{1cm} (4)

where $g$ is the coupling constant.
where \( \mathbb{U} \) is an arbitrary \( 2 \times 2 \) unitary matrix and \( \rho \in \mathbb{R} \) is a parameter with dimension of mass. This is the most general boundary condition, implying the self-adjointness of the operator \(-\partial_x^2\) and thus of the Hamiltonian of the system. The scattering matrix, associated with the point-like interaction generated by (4), is described all possible point-like interactions, which generate a unitary time evolution of \( \psi \). Summarizing, the expectation values (12,13) in the state \( \Omega_{\beta,\mu} \) are exact and satisfy Kirchhoff’s rule. No approximations (like linear response theory) have been used.

The non-equilibrium steady state \( \Omega_{\beta,\mu} \): Following the pioneering work of Landauer and Büttiker, non-equilibrium systems of the type shown in Fig. 1 have been extensively investigated (see [10] and references therein). We use here an algebraic construction [17] of the Landauer-Büttiker (LB) steady state \( \Omega_{\beta,\mu} \) for the problem (2), allowing to establish explicitly the spontaneous breakdown of time-reversal symmetry. Referring for the details to [17], we report only the two-point non-equilibrium correlation function, needed in what follows. Denoting by \( \langle \cdots \rangle_{\beta,\mu} \)the expectation value in the state \( \Omega_{\beta,\mu} \), one has

\[
\langle \psi^*(t_1, x_1, i) \psi(t_2, x_2, j) \rangle_{\beta,\mu} = \int_0^\infty \frac{dk}{2\pi} e^{ikx_1} d_1^\pm(k) d_2^\pm(k) d_3^\pm(k)
\]

which is unitary and satisfies \( S^*(k) = S(-k) \) (Hermitian analyticity) and \( S(\rho) = \mathbb{U} \). Summarizing, the time-reversal symmetry, it turns out [17] that the LB state \( \Omega_{\beta,\mu} \) breaks it down. The simplest way to detect this spontaneous breakdown is to use (3) and observe that

\[
\langle \psi^*(t_1, x_1, i) \psi(t_2, x_2, j) \rangle_{\beta,\mu} \neq \langle \psi^*(-t_2, x_2, j) \psi(-t_1, x_1, i) \rangle_{\beta,\mu},
\]

implying \( T\Omega_{\beta,\mu} \neq \Omega_{\beta,\mu} \). The above argument shows that time-reversal is broken in the LB state \( \Omega_{\beta,\mu} \) independently on the presence or absence of magnetic field or other explicitly breaking terms. This fact should not be surprising because \( \Omega_{\beta,\mu} \) is a non-equilibrium state.

Thermolectric transport in \( \Omega_{\beta,\mu} \): The particle and energy currents are given by

\[
j_x(t, x, i) = \frac{i}{2m} \left[ \psi^*(\partial_x \psi) - (\partial_x \psi^*) \psi \right] (t, x, i),
\]

\[
\theta_{xt}(t, x, i) = \frac{1}{4m} \left[ (\partial_t \psi^*) (\partial_x \psi) + (\partial_x \psi^*) (\partial_t \psi) - (\partial_t \psi^*) \psi - \psi^* (\partial_t \partial_x \psi) \right] (t, x, i).
\]

Inserting (10) into the correlator (6), one gets in the limit \( x_1 \to x_2 = x \) the Landauer-Büttiker expressions

\[
J^N_x = \int_0^\infty \frac{dk}{2\pi m} \sum_{j=1}^2 \left[ \delta_{ij} - |S_{ij}(k)|^2 \right] d_j^\pm(k),
\]

\[
J^E_x = \int_0^\infty \frac{dk}{2\pi m} \sum_{j=1}^n \left[ \delta_{ij} - |S_{ij}(k)|^2 \right] \omega_j(k) d_j^\pm(k).
\]

We stress that the expectation values in the state \( \Omega_{\beta,\mu} \) are exact and satisfy Kirchhoff’s rule. No approximations (like linear response theory) have been used.

Scale invariance: The k-integration in (12,13) with general \( S \)-matrix of the form (4) cannot be performed in closed analytic form. For this reason it is instructive to select among (5) the scale-invariant matrices, which incorporate the universal features of the system while being simple enough to be analyzed explicitly. These so-called critical points of the set (5) are fully classified [10]. One has two isolated points \( S = \pm \mathbb{1} \) and the family

\[
S^U = U \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} U^*, \quad U \in \mathbb{U}(2),
\]

which is the orbit of the matrix \( \text{diag}(1, -1) \) under the adjoint action of the unitary group \( \mathbb{U}(2) \). The transport for \( S = \pm \mathbb{1} \) is trivial because in this case the leads \( L_i \) are actually disconnected. So, we are left with (12) for which the k-integration in (12,13) is easily performed. From now on we consider the Fermi and Bose statistics separately.
Let us derive now the entropy production of the currents. This remarkable simplification allows us to compute the efficiency

\[ \eta = \frac{(\mu_2 - \mu_1) J_1^N}{J_1^Q}, \quad J_1^Q = J_1^E - \mu_1 J_1^N, \]  

where \( J_1^Q \) is the heat current. For this purpose, we assume \( \beta_2 > \beta_1 \) and introduce the variables

\[ \lambda = -\beta \mu_i \quad r = \beta_1 / \beta_2 \in [0, 1]. \]  

Then, using (14), the electric power takes the form

\[ P(\lambda_1, \lambda_2; r; a) = (\mu_2 - \mu_1) J_1^N = \frac{|S_{12}|^2}{2\pi \beta_1} (\lambda_1 - r \lambda_2) \times \left[ \ln \left( 1 + e^{-\lambda_1 - a} \right) - r \ln \left( 1 + e^{-\lambda_2 - a} \right) \right]. \]  

Let us derive now \( \eta(P_{\max}) \). We maximize (19) by varying \( \lambda_1 \) and \( \lambda_2 \) for fixed but arbitrary \( r \) and \( a \). From \( \partial_{\lambda_i} P = \partial_{\lambda_2} P = 0 \) one can deduce that the extrema of (19) are localized at \( \lambda_1 = \lambda_2 \equiv \lambda \), which satisfies the \( r \)-independent equation

\[ \lambda - (1 + e^{\lambda + a}) \ln (1 + e^{-\lambda - a}) = 0. \]  

One can also show that for \( a \in \mathbb{R} \) the equation (20) has a unique solution \( \lambda_0 \), leading to maximal \( P \). Inserting this information in (19), one gets

\[ \eta(P_{\max}) = \frac{(1 - r) \lambda_0 \ln (1 + e^{-\lambda_0 - a})}{(\lambda_0 + a + ar) \ln (1 + e^{-\lambda_0 - a}) - (1 + r) \ln (1 + e^{-\lambda_0 - a})}. \]  

which represents our main result. Notice that \( \eta(P_{\max}) \) vanishes in the isothermal limit \( r \to 1 \).

In order to clarify the role of the parameter \( a \in \mathbb{R} \), we investigate the entropy production

\[ \dot{S} = (\beta_2 - \beta_1) J_1^Q - (\mu_2 - \mu_1) \beta_2 J_1^N. \]  

At maximal power one finds for fermions

\[ \dot{S}(a) = \frac{|S_{12}|^2 (1 + r)(1 - r)^2}{2 \pi r \beta_1} \times \left[ a \ln (1 + e^{-\lambda_0 - a}) - \text{Li}_2 \left( -e^{-\lambda_0 - a} \right) \right], \]  

implying the existence of a point \( a_f = -1.1628... \), such that \( \dot{S}(a) \geq 0 \) for \( a \geq a_f \) and \( \dot{S}(a_f) = 0 \). On the other hand, using (16) and (23), one obtains the following relation between entropy production and energy flow at maximal power

\[ J_1^E(a) = \frac{r}{\beta_1 (1 - r)} \dot{S}(a). \]  

Combining these results with the orientation of the leads \( L_i \) in Fig. 1, we conclude that the energy flow is in the direction 1 \( \to 2 \) for \( a > a_f \) and \( 2 \to 1 \) for \( a < a_f \). Therefore, since \( T_1 > T_2 \), our junction operates as a thermoelectric engine for \( a > a_f \). It turns out that for \( a < a_f = -3.5890... < a_f \) not only the energy flow \( J_1^E \), but also the heat flow \( J_1^Q \) is in the direction \( 2 \to 1 \) (for any \( r \in [0, 1] \)) and thus our devise works as refrigerator.

Let us study in detail the behavior of the junction as a thermoelectric engine. For this purpose one solves numerically the equation (20) for fixed \( a \geq a_f \) and plugs the pair \((a, \lambda_0)\) into (21). The picture, emerging from this analysis, is displayed in Fig. 2. There exists a critical value

\[ a_c = -0.4978... \]  
such that \( \eta_f(P_{\max}) < \eta_{CA} \) for all \( a > a_c \). The conventional Schrödinger junction \( a = 0 \) is in this range. For \( a_f < a < a_c \) one has \( \eta_f(P_{\max}) > \eta_{CA} \) in some interval of \( r \), as shown in Fig. 2 for \( a = -0.7 \). Because of (21) and (23), \( \dot{S}(a_f) = 0 \) implies that \( \eta_f(P_{\max}) \) equals precisely the Carnot efficiency \( \eta_C = 1 - r \) at \( a = a_f \).

From Fig. 2 one can deduce also that the enhancement can be detected in linear response theory (i.e. in the neighborhood of \( r = 1 \)) as well. In fact, for \( a \neq 0 \) the associated Onsager matrix is not symmetric, which is a necessary condition for enhancement above \( \eta_{CA} \).

**Exact efficiency-bosons:** For bosons the computation is totally analogous, except for the presence of a singularity in the integrand of (12) at \( k^2 = -2m(\lambda_i + a)/\beta_i \). In
there exist also leads to maximal

\[ \lambda = (1 - e^{\lambda + a}) \ln(1 - e^{-\lambda - a}) = 0, \quad \lambda + a > 0, \quad (25) \]

\[ \eta_b(P_{\text{max}}) = \frac{(1 - r)\lambda_a \ln (1 - e^{-\lambda_a - a})}{(\lambda_a + a + ar) \ln (1 - e^{-\lambda_a - a}) - (1 + r)\ln(e^{-\lambda_a - a})}, \quad (26) \]

where \( \lambda_a \) satisfies \( (25) \). The study of equation \( (25) \) shows that for \( a < a_b \) there is no (real) solution for \( \lambda \). There is one solution of \( (25) \) for \( a = a_b \), which is a saddle point of the power \( P \). In the interval \( a_b < a \leq 0 \) there are two solutions, one of which being a maximum of \( P \). Finally, for \( a > 0 \) there is one solution, which also leads to maximal \( P \). Summarizing, for each \( a > a_b \) there exist \( \lambda_a \) satisfying both conditions \( (25) \) and giving a maximal power. Moreover, the entropy production \( (22) \) for bosons is positive in this range.

For illustration we have plotted in Fig. 3 the efficiency \( \eta_b(P_{\text{max}}) \) for some values of the control parameter \( a \). It turns out that \( \eta_b(P_{\text{max}}) \) never exceeds \( \eta_{CA} \) in the allowed domain \( a > a_b \). At maximal power the bosonic junctions behave therefore differently from the fermionic ones. We stress that the condition \( (25) \) is essential for this conclusion. If we release this condition, there exist points in the \( (a, \lambda) \)-plane (e.g. \( (a = -1, \lambda = 28) \)) with positive entropy production, in which also the bosonic efficiency becomes larger then \( \eta_{CA} \) and approaches \( \eta_C \). However the power, delivered in these points, is not maximal.

Comparison with other bounds: For classical engines, which can reach the Carnot efficiency \( \eta_C \) in the reversible limit, the following upper and lower bounds

\[ \frac{1}{2} \eta_C \equiv \eta_- \leq \eta(P_{\text{max}}) \leq \eta_+ \equiv \frac{\eta_C}{2 - \eta_C}, \quad (27) \]

have been established in \( [20, 22] \) without referring to linear response theory. For comparison with the CA bound we observe that \( \eta_- \leq \eta_{CA} \leq \eta_+ \). Since \( \eta_f(P_{\text{max}}) = \eta_C \) for \( a = a_f \), the fermion efficiency exceeds for appropriate values of \( a \) not only \( \eta_{CA} \), but also \( \eta_+ \). For bosonic junctions one has instead \( \eta_b(P_{\text{max}}) < \eta_- \) for all allowed \( a \geq a_b \), as illustrated in Fig. 4.

Conclusions: We derived and analyzed systematically the exact efficiency \( \eta(P_{\text{max}}) \) for critical Schrödinger junctions in the Landauer-Büttiker steady state. Provided that the transmission probability between the two reservoirs does not vanish, the intensity of the interaction in the junction is irrelevant for \( \eta(P_{\text{max}}) \) in the critical regime. Quantum irreversibility is implemented in our framework by a spontaneous breaking of time-reversal symmetry. We discovered that such a breaking is compatible with vanishing entropy production for certain value of the parameter \( a \). In fact, in the fermion case \( S(a_f) = 0 \), implying that \( \eta_f(P_{\text{max}}) \) reaches the Carnot efficiency. The same mechanism works for bosons as well, but the corresponding value of \( a \) in this case is not in the regime of maximal power. Further clarifying the role of the parameter \( a \) and its impact on other physical observables (maximal efficiency, quantum noise,...) represents an interesting subject for future investigations.

\[ \text{FIG. 3: (Color online) The CA bound (continuous red line) compared to } \eta_b(P_{\text{max}}) \text{ for the same values of } a \text{ as in Fig. 4}\]

\[ \text{FIG. 4: (Color online) The } \eta_f \text{ bounds (continuous red line) compared to } \eta_f(P_{\text{max}}) \text{ for the same values of } a \text{ as in Fig. 4} \]

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