Statistical analysis of the figure of merit of a two-level thermoelectric system: a random matrix approach

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Abstract – Using the tools of random matrix theory we develop a statistical analysis of the transport properties of thermoelectric low-dimensional systems made of two electron reservoirs set at different temperatures and chemical potentials, and connected through a low-density-of-states two-level quantum dot that acts as a conducting chaotic cavity. Our exact treatment of the chaotic behavior in such devices lies on the scattering matrix formalism and yields analytical expressions for the joint probability distribution functions of the Seebeck coefficient and the transmission profile, as well as the marginal distributions, at arbitrary Fermi energy. The scattering matrices belong to circular ensembles which we sample to numerically compute the transmission function, the Seebeck coefficient, and their relationship. The exact transport coefficients probability distributions are found to be highly non-Gaussian for small numbers of conduction modes, and the analytical and numerical results are in excellent agreement. The system performance is also studied, and we find that the optimum performance is obtained for half-transparent quantum dots; further, this optimum may be enhanced for systems with few conduction modes.

Introduction. – Low-dimensional systems offer a wealth of technological possibilities thanks to the rich variety of artificial custom-made semiconductor-based structures that nowadays may be routinely produced. The properties of these systems, including confinement geometry, density of states, and band structure, may be tailored on demand to control the transport of heat and confined electrical charges as well as their coupling. This is crucial to further improve the performance and increase the range of operation of current thermoelectric devices.

From a thermodynamic viewpoint, thermoelectric systems connected to two thermal baths at temperatures $T_{\text{hot}}$ and $T_{\text{cold}}$, use their conduction electrons as a working fluid to directly convert a heat flux into electrical power and vice-versa with efficiency $\eta$. As for all heat engines, one seeks to increase $\eta$, the maximum of which, $\eta_{\text{max}}$, is related to the figure of merit of the system $ZT$:

$$\eta_{\text{max}} = \eta_C \frac{\sqrt{1 + ZT} - 1}{\sqrt{1 + ZT + T_{\text{cold}}/T_{\text{hot}}}}$$

where $\eta_C = 1 - T_{\text{cold}}/T_{\text{hot}}$ is the Carnot efficiency. In the frame of linear response theory, the figure of merit may be expressed as: $ZT = \sigma S^2 T/\kappa$, where $S$ is the thermopower, $T$ is the average temperature across the device, and $\sigma$ and $\kappa$ are the electrical and thermal conductivities respectively, with $\kappa = \kappa_e + \kappa_{\text{lat}}$, accounting for both electron and lattice thermal conductivities. Equation (1) thus clearly shows that for given working conditions, $ZT$ is as good a device performance measure as the efficiency $\eta$ is.

Quantum dots may be defined as confined electronic systems whose characteristic size is much smaller than the electron mean free path; the size and shape of the region where electrons are confined are controlled by gates. Amongst the various low-dimensional thermoelectric systems that have been studied, quantum dots keep attracting much interest because of their narrow, Dirac-like, electron transport distribution functions or, equivalently, sharply peaked energy-dependent transmission profiles $T$, which permit obtainment of extremely high values of elec-
tronic contribution to $ZT$ \cite{4}. There is a simple relationship between the electrical conductivity $\sigma$ appearing in the definition of the figure of merit and the transmission function $T$: $\sigma = (2e^2/h)T$, the proportionality factor being the quantum of conductance ($e$ is the electron charge, and $h$, Planck’s constant).

The treatment of confined systems may be achieved, without loss of pertinence, by means of very simple models such as, e.g., the resonant level model of thermal effects in a quantum point contact \cite{5} and the two-level model of a mesoscopic superconductor \cite{6}, which capture the essential physics of the actual systems. The use of non-interacting two-level model systems for quantum dots or very small electronic cavities may be justified if these are strongly coupled to the reservoirs, i.e. if the confinement yields a mean level spacing that is large \cite{7} compared to the charging energy $e^2/C$, $C$ being the capacitance of the dot \cite{8,9}. These models also are justified for probing the spectrum edges of mesoscopic systems \cite{10,11} where the physics is different from that of the bulk spectrum \cite{10,12}.

If one of the gates generates a random potential, the quantum dot behaves as a chaotic cavity; measurements of thermopower and analysis of its fluctuations \cite{13} demonstrated the non-Gaussian character of the distribution of thermopower consisting of negatively charged top gates (yellow) on a two dimensional electron gas. The potential on the right three top gates may be varied randomly in order to slightly modify the shape of the cavity and therefore obtain a statistical ensemble \cite{13}. The red (blue) part represents the hot (cold) electronic reservoir connected to the cavity. The inset shows the system as modeled by the Hamiltonian.

Fig. 1: (Colour on-line) Schematic figure of the two level system quantized electron creation and annihilation operators in the state $k$. The two energy levels and their coupling are characterized by the Hamiltonian $H_s$:

$$H_s = \begin{pmatrix} v_1 & v_{12} \\ v_{21} & v_2 \end{pmatrix}$$

where the on-site potentials $v_1, v_2$ and the coupling $v_{12}$ are chosen to be random to describe the chaotic behavior of the system. We assume that the left (right) lead is only connected to the site $v_1 (v_2)$. The contribution $H_c$ involves the coupling matrix $W$ entering the definition of the scattering matrix \cite{18}:

$$S = 1 - 2\pi i W^\dagger \frac{1}{\epsilon - H_s - \sum} W$$

where $\Sigma$ is the self-energy of the two leads. To keep our analysis on a general level, we only give its form: $\Sigma = \Lambda - i\pi WW^\dagger$, with $\Lambda$ being the real part. With the assumption of symmetric reservoirs, the self-energy is proportional to the identity, in which case $W = \sqrt{\Gamma/2\pi I_{2 \times 2}}$, where $\Gamma = -2\Sigma$ characterizes the broadening. Throughout the Letter, we adopt the same notations for scalars and their corresponding matrix form when this latter is proportional to the identity.

The scattering matrix $S$ is unitary. In the absence of a magnetic field, time reversal symmetry is preserved and the matrix $S$ is therefore symmetric, which implies $v_{12} = v_{21}$.
$v_{21}$. Moreover, for simplicity, we consider in the first part of this Letter, systems with left-right spatial symmetry ($v_1 = v_2$), so that the reflection from left is the same as that from right. The matrix $S$ may thus read:

$$S = \begin{pmatrix} r & t \\ t & r \end{pmatrix}$$  \quad (4)$$

where $r$ and $t$ are the reflection and transmission amplitudes respectively. With these definitions, the transmission of the system and the Seebeck coefficient read:

$$T = |t|^2, \quad S = \frac{\partial \ln(T)}{\partial \epsilon}$$  \quad (5)$$

The Seebeck coefficient is obtained at low temperatures with the Cutler-Mott formula \[19\]. Here, it is expressed in units of $\frac{e}{3k_B T}$ (omitting the sign). The transmission of the system can then be directly obtained using the Fisher-Lee formula \[20\]:

$$T = \Gamma G_{12} \Gamma G_{12}^\dagger$$  \quad (6)$$

where the off-diagonal element of the Green’s matrix is $G_{12} = \frac{1}{4} \frac{(\epsilon_1 - \epsilon_2)}{(|\epsilon - \epsilon_1 - \Sigma|(|\epsilon - \epsilon_2 - \Sigma)|^2)}$, with $\epsilon_1$ and $\epsilon_2$, eigenvalues of $\mathcal{H}_u$. And, we may thus write:

$$T(\epsilon) = \frac{\Gamma^2}{4} \frac{(\epsilon_1 - \epsilon_2)^2}{(|\epsilon - \epsilon_1 - \Sigma|(|\epsilon - \epsilon_2 - \Sigma)|^2)}$$  \quad (7)$$

which is valid if the left/right symmetry is satisfied. Now, combination of Eqs. (5) and (7) yields an expression of the Seebeck coefficient containing the scattering matrix $S$:

$$S = \frac{\alpha}{2} \text{Tr} \left( \frac{e^{i\Theta} S - e^{-i\Theta} S^\dagger}{2i} \right)$$  \quad (8)$$

with $\alpha = 4|1 - \Sigma|/\Gamma$, $\Theta = \text{Arg}(1 - \Sigma)$, and $\Sigma = \partial_\epsilon \Sigma$. For an energy $\epsilon = \epsilon_0$, which corresponds in general to the middle of the conduction band of a semi-infinite lead (or half-filling limit), the imaginary part of the self-energy derivative vanishes: $3\Sigma(\epsilon_0) = 0$. We stress that Eq. (8) may also be derived if the constraint on left-right symmetry is relaxed, and that it constitutes an important result upon which all the subsequent statistical analysis is based.

**Statistics of the Seebeck coefficient.** In this work, the scattering matrix $S$ is a random variable, which we assume to be uniformly distributed; hence $S$ belongs to circular orthogonal ensembles (COE) \[21\]. The statistics of the Seebeck coefficient thus follows:

$$P_c(S) = \int \delta \left\{ S - \frac{\alpha}{2} \text{Tr} \left( \frac{e^{i\Theta} S - e^{-i\Theta} S^\dagger}{2i} \right) \right\} \delta S$$  \quad (9)$$

The Haar measure $\delta S$ is invariant under the transformation $S \rightarrow VSV^T$ for any arbitrary unitary matrix $V$ (the superscript $^T$ denotes the transpose of a matrix). With $V = e^{i\Theta}/\Gamma_{12 \times 2}$, we obtain:

$$P_c(S) = \int \delta \left\{ S - \frac{\alpha}{2} \text{Tr} \left( \frac{\delta - \delta^\dagger}{2i} \right) \right\} \delta S = \frac{1}{\alpha} P_{c=\epsilon_0}(S/\alpha)$$  \quad (10)$$

where $\alpha = \alpha/\alpha_0$ with $\alpha_0 = \alpha(\epsilon_0)$. Equation (10) shows that the general probability distribution of the Seebeck coefficient at arbitrary energy can be deduced directly from the simpler one obtained at $\epsilon_0$.

Note that for ease of notations, we retain $P$ as a generic notation for all the probability distributions in the subsequent parts of the letter.

**Joint probability distribution function.** A similar analysis of the transmission $T$ shows that its distribution does not depend on energy \[22\]. Since the transport coefficient $T$ and $S$ are tightly related by the transport equations, we need the joint probability distribution (j.p.d.f) $P_c(T,S)$ to study any observable depending on both $T$ and $S$. The starting point for this is the rewriting of the scattering matrix using the following decomposition:

$$S = R^2 \left( \begin{array}{cc} e^{i\Theta_1} & 0 \\ 0 & e^{i\Theta_2} \end{array} \right) R$$  \quad (11)$$

where the rotation matrix $R$ is defined as:

$$R = \frac{1}{\sqrt{2}} \left( \begin{array}{cc} 1 & -1 \\ 1 & 1 \end{array} \right)$$  \quad (12)$$

The eigenphases $\theta_1$ and $\theta_2$ are independent and uniformly distributed in $[-\pi, +\pi]$ which is the consequence of $S$ being taken from COE with the left-right symmetry \[24\]. Now, we analyze the j.p.d.f. of the Seebeck coefficient and transmission at the half-filling limit $\epsilon = \epsilon_0$ \[25\], with:

$$T = \sin^2 [(\theta_1 - \theta_2)/2]$$  \quad (13)$$

and

$$S = \alpha_0 \sin [(\theta_1 + \theta_2)/2] \cos [(\theta_1 - \theta_2)/2]$$  \quad (14)$$

The j.p.d.f. may now take the form:

$$P_{c=\epsilon_0}(S,T) = \langle \delta (T - \sin^2 u) \delta (S - \alpha_0 \sin v \cos u) \rangle_{u,v}$$  \quad (15)$$

where two independent and uniformly distributed variables $u = \frac{\theta_1 - \theta_2}{2\pi}$ and $v = \frac{\theta_1 + \theta_2}{2\pi}$ are introduced. Integration over these variables and use of Eq. (10) yield:

$$P_c(S,T) = \frac{1}{\pi \sqrt{T(1-T)}} \int \frac{1}{\pi \alpha^2(1-T) - S^2}$$  \quad (16)$$

which constitutes one of the main results of this work since it shows the possible values of the couple $(S,T)$: $P_c(S,T)$ is non-zero only if the following condition is satisfied:

$$\alpha^2(1-T) - S^2 > 0, \quad T < 1$$  \quad (17)$$

The relationship between the Seebeck coefficient and the transmission function is thus constrained by a parabolic law. This may be checked by sampling the $S$ matrices belonging to the COE with the left/right symmetry, from which the transport coefficients $T$ and $S$ are numerically computed with Eqs. (5) and (8). The parabolic law is clearly shown on Fig. 2 where the j.p.d.f. $P_c(S,T)$ is plotted against $T$ and $S$. 

p-3
To study the system performance, we compute the figure of merit $Z T$ whose maximum is reached when the power factor $p = T S^2$ is reached. Satisfaction of this latter condition lies on the existence of the probability $P_e(T, S)$:

$$
\alpha(1 - T) - S^2 > 0 \implies \alpha(T(1 - T) > TS^2
\implies \max(\alpha T(1 - T)) > p \implies \alpha/4 > p
$$

We thus find that $Z T$ reaches its maximum if the transmission $T = \frac{1}{2}$. Physically, this means that the best performance results from the conditions that make the system half-transparent; this is numerically checked on Fig. 2.

**Marginal distributions.** The marginal distributions $P_e(T)$ and $P_e(S)$ are obtained from the integration of $P_e(S, T)$ over $S$ and $T$ respectively:

$$
P_e(T) = \frac{1}{\pi} \sqrt{\frac{1}{1 - T}}
$$

$$
P_e(S) = \frac{2}{\alpha \pi} K \left(\sqrt{1 - S^2/\alpha^2}\right)
$$

where $K$ is the complete elliptic integral of the first kind. It is interesting to note that $P_e(T)$ does not depend on the energy since it derives from the sole assumption that the scattering matrix is uniformly distributed (Dyson’s CE) with the left/right spatial symmetry [24]. As for all the physical observables with no energy derivative in their expression (shot noise for example), their distributions do not depend on the number of levels $N$ in the system: for all $N \geq 2$, we obtain the same distribution, as it can be seen with the decimation method [11, 15] as on the condition that $S \in \{\text{CE}\}$.

The case of the Seebeck coefficient is different: its distribution $P_e(S)$ depends on the number of levels in the system since its expression contains an energy derivative. The only situation where the Seebeck coefficient, scaled with the appropriate parameter ($\alpha$ in our case), is independent on the number of levels is at the edge of the Hamiltonian spectrum [10] where the result can be obtained by assuming the simpler two-level system considered as the minimal cavity for the two-mode scattering problem [11].

All the results presented so far in this Letter were obtained and discussed assuming a two-level system with left/right spatial symmetry and $S \in \{\text{CE}\}$. We must now see whether these hold when the assumption of left/right spatial symmetry is relaxed.

**Relaxation of the spatial symmetry assumption.** Assuming that there is no left/right symmetry, the two eigenphases $\theta_1$ and $\theta_2$ of Eq. [11] are no longer independent, and we must consider a distribution of the form:

$$
P_e(\theta_1, \theta_2) \propto |e^{i\theta_1} - e^{i\theta_2}|^{24}.
$$

The treatment is the same as for the previous case, and while we obtain a different j.p.d.f. for the Seebeck and the transmission coefficients:

$$
P_e(T, S) = \frac{1}{\alpha \pi^2} \frac{1}{\sqrt{1/(1 - T)}} K \left(\sqrt{1 - S^2/\alpha^2}(1 - T)\right)
$$

the mathematical constraint on the couples $(T, S)$ to obtain a non-vanishing joint probability distribution is exactly the same as Eq. [18]; this implies that the best system performance is obtained when it is half-transparent: $T = \frac{1}{2}$.

The marginal distributions of $S$ and $T$ are also different:

$$
P_e(T) = \frac{1}{2\sqrt{T}}
$$

$$
P_e(S) = -\frac{1}{\alpha \pi} \ln \left(\frac{|S|/\alpha}{1 + \sqrt{1 - S^2/\alpha^2}}\right)
$$

Equation [22] is consistent with results of Refs. [26, 27] obtained with different methods and Eq. [23] confirms the result of [10]. We see in both distributions, Eqs. [16] and [21], that the variables $(T, S)$ are not independent but it is interesting to note that if we define a new variable $X = S/\sqrt{(1 - T)}$ then we have two independent variables, and the j.p.d.f. becomes multiplicatively separable:

$$
P_e(T, X) = P_e(T) \times P_e(X)
$$

where we have $P_e(X) = 1/\pi \sqrt{\alpha^2 - X^2}$ in the symmetric case and $P_e(X) = \frac{\alpha X}{\pi \sqrt{1 - X^2/\alpha^2}}$ when the symmetry is relaxed; $P_e(T)$, given above, is the corresponding marginal distribution. It is worth mentioning that $S$ and $X$ also constitute a couple of independent variables.

**Discussion.**

**Seebeck coefficient and density of states.** The local density of states in the central system, when connected to
The number of energy levels in the cavity equals the total number of modes. In the inset, the standard deviation of the power factor is shown as a function of $M$. The results are fitted with the function $\sqrt{\delta p^2} \sim 0.08/M$. The numerical results are obtained by sampling $2.1 \times 10^5$ scattering matrices.

The leads \(^2\), reads:

$$\rho(\epsilon) = -\frac{1}{\pi} \Im \text{Tr} \frac{1}{\epsilon - H_s - \Sigma}$$

(25)

which combined with Eq. (25) yields:

$$\frac{\delta \rho(\epsilon)}{\bar{\rho}(\epsilon)} = \frac{1}{2} \text{Tr} \left( \frac{S + S^\dagger}{2} \right)$$

(26)

where $\delta \rho = \rho - \bar{\rho}$ and $\bar{\rho}(\epsilon) = 2/\pi \Gamma$. The analysis of this expression shows that the relative change in the density of states differs from the Seebeck coefficient, Eq. (8), but the interesting result is that both $\delta \rho(\epsilon)/\bar{\rho}(\epsilon)$ and $S/\alpha$ have exactly the same distribution, which may be seen by using the invariance of the Haar measure under the transformation $S \rightarrow -i\Sigma$. We finally add to this set of variables the scaled Wigner time $\delta \tau_w/\alpha$ which is related to the time spent by a wavepacket in the scattering region: $\tau_w = -i\hbar \text{Tr}(S^\dagger \partial S/\partial \epsilon)$ \(^1\).

Generalisation to $M$ modes of conduction. Here, we generalise and investigate the performance of a system with a large number of conduction modes. We concentrate on systems with $2N$ levels connected to $2M$ independent and equivalent leads ($M$ from the left side and $M$ from the right side). We suppose that the number of modes $M$ is the same as the number of levels: $M = N$. This case is pertinent because it corresponds to the model of minimal chaotic cavities, which gives the same results as for the general case $N > M$ at the edge of the spectrum \(^1\). We also assume no spatial symmetry.

The form of the scattering matrix which is now of size $2M \times 2M$ remains unchanged [see Eq. (3)], and the transmission is given by $T = \text{Tr}(t^\dagger t)$. For large numbers of modes, the shape of p.d.f. of the transmission tends to that of a Gaussian distribution for the typical values of $T$ around its mean which for $M$ large is given by $T \sim M/2$. The variance of this Gaussian is equal to $(\delta T^2) = 1/8$ which does not depend on $M$ because of the universal character of the conductance fluctuations \(^1\). It is worth mentioning that the tail of the distribution, which describes the atypical values of the conductance has a non-Gaussian form \(^3\). At first glance, this scaling of the mean transmission seems to favour an enhancement of the power factor and hence of the figure of merit; however, our study of the Seebeck coefficient yields a different conclusion as we now explain.

The Seebeck coefficient may be expressed by writing the derivative of the scattering matrix and using the expression $S = 2\Re(\text{Tr}(it^\dagger)/T)$ (where the dot refers to the energy derivative and $\Re$ is the real part); then it is computed numerically assuming modes with a self-energy $\Sigma = \epsilon/2 - i\sqrt{1 - (\epsilon/2)^2}$ \(^3\). Still considering the half filling limit since the generalisation to arbitrary energy presents no particular difficulty, we find that the mean value of the Seebeck coefficient is always zero: $\langle S \rangle = 0$ because the probability to obtain a positive thermopower is the same as that for a negative coefficient. The most interesting result is the standard deviation which appears to scale as: $(\delta S^2)^{1/2} = O(1/M)$. This clearly demonstrates that increasing the number of conduction modes in the system induces a decrease of the thermopower as shown in Fig. 4 where the standard deviation of thermopower is represented as a function of the number of modes on each side (left and right). The numerical results were obtained by sampling scattering matrices of size $2M \times 2M$ from the circular orthogonal ensemble and computing a histogram from which the standard deviation was obtained.

Since $p \propto S^2$, the lowering of the system performance induced by a decrease of the thermopower, which is faster...
than the increase due to conductance, is a reflection of the fact that the typical power factor is thus estimated to scale as $1/M$. We deduce from this analysis that the distributions $\mathcal{P}(T - \bar{T})$ and $\mathcal{P}(MS/\alpha)$ do not depend on $M$ for large values of $M$. In Fig. 5, we see a very good agreement between the distribution $\mathcal{P}(MS/\alpha)$ and the Gaussian centered on zero. We also see from the j.p.d.f of $ZT$ and $T$ that high values of the figure of merit are obtained for $T \sim M/2$, which generalises the result obtained for the two-level system.

Concluding remarks. – We investigated the quantum thermoelectric transport of nanosystems made of two electron reservoirs connected through a low-density-of-states two-level chaotic quantum dot, using a statistical approach. Analytical expressions based on an exact treatment of the chaotic behavior in such devices were obtained and analyzed to provide the conditions for optimum performance of the system. We find that the optimum efficiency is obtained for half-transparent dots; this optimum may be enhanced for systems with few conducting modes, for which the exact transport coefficients probability distributions are found to be highly non-Gaussian.

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