Quantum vs. stochastic non-equilibrium steady state of sparse systems

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A resistor-network picture of transitions is appropriate for the study of energy absorption by weakly chaotic or weakly interacting driven systems. Such "sparse" systems reach a novel non-equilibrium steady state (NESS) once coupled to a bath. In the stochastic case there is an analogy to the physics of percolating glassy systems, and an extension of the fluctuation-dissipation phenomenology is proposed. In the mesoscopic case the quantum NESS might differ enormously from the stochastic NESS, with saturation temperature determined by the sparsity. A toy model where the sparsity of the system is modeled using a log-normal random ensemble is analyzed.

The study of systems with non-equilibrium steady state (NESS) has become of great interest in recent years [1–7]. Attempts to introduce various generalizations of linear response theory (LRT) are sometimes entitled "extension" or "violation" of the fluctuation-dissipation relation theorem (FDT) [8–14]. The paradigm for NESS is a system that is coupled to two equilibrated reservoirs, "A" and "B", which are characterized by spectral functions $\tilde{S}_A(\omega)$ and $\tilde{S}_B(\omega)$. Each reservoir satisfies the detailed balance condition

$$\frac{\tilde{S}(\omega)}{\tilde{S}(-\omega)} = \exp\left(-\frac{\omega}{T}\right) \tag{1}$$

but with different temperatures T_A and T_B. Hence the NESS of the system is not canonical, and it cannot be characterized by an equilibrium temperature. A particular case of special interest is obtained if one reservoir (call it "A") is replaced by a stationary driving source, while the relaxation is provided by a bath (call it "B") that has some finite temperature T_B. This is still the same paradigm because formally the driving source "A" can be regarded as a bath that has an infinite temperature $T_A = \infty$ hence $\tilde{S}_A(-\omega) = \tilde{S}_A(\omega)$.

Novel NESS.– In recent studies [15–18], we have suggested that there is a class of systems for which the rate of energy absorption is a semi-linear rather than a linear functional with respect to $\tilde{S}_A(\omega)$. This theory, termed semi-linear response theory (SLRT), is based on a resistor network picture of the transitions between energy levels (Fig.1). Due to the percolation-like nature of the dynamics, SLRT typically predicts a suppressed rate of heating compared with LRT. In previous SLRT publications, the effect of the surrounding environment has been neglected, and it has been conjectured that weak coupling to a bath would lead to a non-canonical NESS. Consequently, the expectation is to have, for strong driving, a crossover from an LRT canonical-like NESS to a novel non-canonical NESS, with the possibility of remarkable quantum-mechanical fingerprints.

LRT phenomenology.– Under the assumptions of very weak driving, and that all the driven transitions have comparable rates $\approx w$, one may reason that the system is in a canonical-like state with some temperature T. From the phenomenological rate equation it follows that the driving induces diffusion $D \propto w$ in energy space [19–23], leading to a rate of heating

$$\dot{W} = \frac{D}{T} \tag{2}$$

Similarly it is straightforward to show (see supplementary material), that the rate of cooling due to the interaction with the bath can be written as

$$\dot{Q} = \frac{D_B}{T_B} - \frac{D_B}{T} \tag{3}$$

where the first term is due to the imbalance of upward and downward transition rates, while the second term is due to the non-uniformity of the probability distribution in energy space. At steady state $\dot{W} = \dot{Q}$, so a phenomenological determination of the steady state temperature T is possible.

SLRT phenomenology.– Let us consider a quasi-continuum of energy levels E_n that have level spacing Δ_0, and assume that the bath and the driving induce near-neighbor transitions only. The bath induced downward and upward transition rates are $w_\beta e^{\pm\Delta_0/(2T_B)}$, with $T_B \gg \Delta_0$, where w_β is a constant related to the strength of the coupling. On the other hand, the driving induced transition rates w_n are characterized by a logarithmically wide (say log-normal) distribution, which is typical in the case of, e.g., weakly chaotic systems. Consequently, the bath induced diffusion has the coefficient $D_B = w_\beta \Delta_0^2$, while for the driving induced diffusion

$$D_{[\mathrm{LRT}]} = \overline{w_n}\,\Delta_0^2 \tag{4}$$

$$D_{[\mathrm{SLRT}]} = [\overline{1/w_n}]^{-1}\,\Delta_0^2 \tag{5}$$

where the LRT result is based on the traditional Kubo formalism, while the SLRT prediction reflects a network that consists of resistors that are connected in series (see Fig.1 for illustration). Accordingly it is expected that the steady state temperature for *strong* driving would be $T_{[\mathrm{SLRT}]} = [\overline{w_\beta/w_n}]^{-1} T_B$, i.e. much lower compared with the Kubo-implied naive expectation $T \approx [\overline{w_n/w_\beta}] T_B$.

Modeling.– It should be clear that SLRT applies whenever the transport is modeled using a resistor net-

work. Thus it might have applications, e.g., in statistical mechanics and biophysics. But the original motivation for SLRT came from mesoscopics, where the quantum nature of reality cannot be ignored. In this context the Hamiltonian contains a driving term $f(t)W$, and the transition rates $w_{nm} \propto |W_{nm}|^2$ between levels are determined by the Fermi-Golden-Rule (FGR). For weakly chaotic or weakly interacting systems W_{nm} is typically sparse and textured, and hence SLRT seems to be of relevance. In order to avoid repetition, we define the quantum model, and regard the classical model as a special case. Assuming that $f(t)$ has the correlation function $\langle f(t)f(t')\rangle = \varepsilon^2\delta(t-t')$, the master equation is

$$\frac{d\rho}{dt} = -i[\mathcal{H}_0,\rho] - \frac{\varepsilon^2}{2}[W,[W,\rho]] + \boldsymbol{\mathcal{W}}^{\beta}\rho \tag{6}$$

In the energy basis, $\mathcal{H}_0$ is a diagonal matrix with energy levels E_n. The state of the system is represented by the probability matrix, which can be rewritten as a column vector $\rho \mapsto (p_n;\rho_{\nu\mu})$, composed of the diagonal *probabilities* and the off-diagonal *coherences*. Consequently, the master equation takes the form $\dot{\rho} = \boldsymbol{\mathcal{W}}\rho$ where

$$\boldsymbol{\mathcal{W}} = \begin{pmatrix} \mathcal{W} & \Lambda^{\dagger} \\ \Lambda & \mathcal{W}^{\perp} \end{pmatrix} \tag{7}$$

The definition of Λ is implied by the second term in Eq.(6). The diagonal blocks have contributions also from the bath term $\boldsymbol{\mathcal{W}}^{\beta}$. In particular

$$\mathcal{W}_{mn} = w_{mn} + w^{\beta}_{mn}\,\mathrm{e}^{(E_n-E_m)/(2T_B)} \tag{8}$$

$$\mathcal{W}_{nn} = -\Gamma_n \tag{9}$$

$$\mathcal{W}^{\perp}_{\nu\mu,\nu\mu} = i\Delta_{\nu\mu} - \gamma_{\nu\mu} - \gamma_{\beta} \tag{10}$$

$$\Lambda_{n,\nu\mu} = \varepsilon^2 W_{n\nu}W_{\mu n}, \quad \text{for } \nu,\mu \neq n \tag{11}$$

where $w_{nm} = \varepsilon^2|W_{nm}|^2$ and w^{β}_{nm} are symmetric matrices, and $\mathcal{W}_{mn}$ is the transition rate from n to $m(\neq n)$, and Γ_n is the associated decay rate as implied by conservation of probability. We use the notations $\Delta_{nm} = E_n - E_m$, and $\gamma_{\nu\mu} = (\varepsilon^2/2)[(W^2)_{\nu\nu}+(W^2)_{\mu\mu}]$. For simplicity, we assume that the bath induced dephasing γ_{β} is the same for all the coherences. For the near-neighbor transitions model, we simplify the subscripts and write, e.g., w_n instead of $w_{n,n-1}$.

Numerics.– In the simulations, we have N=25 levels, with equal level spacing Δ_0=1. The bath temperature is T_B=10. The bath induced transition rates are taken as $w_{\beta} = 10^4$. The driving induced transition rates are log normally distributed. Namely, $w = \exp(x)$, where x has a Gaussian distribution with average μ and dispersion σ that are determined such that the driving intensity is $\langle w\rangle = \varepsilon^2$, and the sparsity [18] is $s = \exp(-\sigma^2)$. The value $s \sim 1$ means that all the elements are comparable and well represented by their average. Sparsity means $s \ll 1$, for which the median differs by orders of magnitude from the algebraic average.

NESS determination.– The steady state solution satisfies the equation $\boldsymbol{\mathcal{W}}\rho = 0$, from which the NESS occupation probabilities p_n are determined, as as in Fig.2. From this one can extract the NESS heating rate as in Fig.3. In the absence of driving, the steady state is canonical with a well-defined temperature T_B. In the presence of driving, the state is generally not canonical. Consequently, we can formally define a different microscopic temperature T_{nm} for each pair of coupled levels via

$$\frac{p_n}{p_m} = \exp\left(-\frac{E_n - E_m}{T_{nm}}\right) \tag{12}$$

For a model with near-neighbor transitions, we use the simpler indexing T_n. We define the NESS temperature (Fig. 4) as the harmonic average over T_n, which means that $1/T$ is the average over $1/T_n$.

Stochastic NESS.– In the stochastic case, i.e. Eq.(7) with $\Lambda = 0$, the master equation become a simple rate equation, from which it follows that the temperature of the n*th* transition is $T_n = [(w_n+w_{\beta})/w_{\beta}]T_B$, and the NESS temperature is

$$T = \left[\overline{\left(\frac{1}{T_n}\right)}\right]^{-1} = \left[\overline{\left(\frac{w_{\beta}}{w_{\beta}+w_n}\right)}\right]^{-1} T_B \tag{13}$$

With this definition one can easily prove that Eq.(3) still holds, while the expression for the energy absorption is

$$\dot{W} = \left[\overline{\left(\frac{w_n}{w_{\beta}+w_n}\right)}\right]\frac{D_B}{T_B} \tag{14}$$

Defining the steady state diffusion coefficient D from the relation $\dot{W} = D/T$ we get

$$D = \left[\overline{\left(\frac{w_n}{w_{\beta}+w_n}\right)}\right]\left[\overline{\left(\frac{1}{w_{\beta}+w_n}\right)}\right]^{-1}\Delta_0^2 \tag{15}$$

One realizes that if all the w_n are comparable, then $D \approx D_{[\mathrm{LRT}]} \approx D_{[\mathrm{SLRT}]}$. But if the w_n have a log-wide distribution, the agreement with LRT is achieved only if the w_n are all much smaller than w_{β}. For strong driving, both D and T are $\propto [\overline{1/w_n}]^{-1}$, as expected from the SLRT phenomenology, while their ratio approaches the bath limited value $\dot{W}_{\infty} = D_B/T_B$.

Quantum NESS.– The stochastic FGR picture applies if the off-diagonal terms become negligible. By inspection, there are two small parameters involved: One possibility is that the transition rates w are much slower compared with the environmentally induced dephasing γ_{β}. The second possibility is to have w much smaller compared with the level spacing Δ_0. The latter is the traditional assumption in atomic physics, and can be regarded as "microscopic circumstances". But in "mesoscopic circumstances" Δ_0 might be small, and the validity of FGR is not guaranteed.

Turning to the numerics (e.g., Fig.3), we observe that in mesoscopic circumstances, if the environmentally induced dephasing γ_β is neglected, the quantum NESS departs from the classical NESS as the driving intensity is increased. The sparsity of the system is characterized by a parameter $s \ll 1$ that reflects so to say [18] the percentage of the large elements. While both LRT and SLRT predict an unbounded increase of the temperature as the driving becomes stronger, the quantum NESS exhibits saturation (see Fig.4), which is characterized by a finite temperature that we call T_∞.

One would like to understand how T_∞ emerges. For this purpose we point out that one can adopt a Fokker-Planck interpretation of the master equation, where n is like the momentum. In the absence of sparsity, W is like the position coordinate, and its eigenstates are extended in n. But if $s \ll 1$, then W is like (off-diagonal) disorder, and its eigenstates r become localized in n, with energies $\langle E\rangle_r$ that are no longer identical. It is clear that if the driving is very strong, the NESS becomes a mixture of the eigenstates r. Some further argumentation implies that the weights p_r should be similar to $\exp(-\langle E\rangle_r/T_B)$. For s=1 (which is like no disorder), all the $\langle E\rangle_r$ are the same, and therefore the p_r and hence the p_n distribution is uniform, corresponding to $T_\infty = \infty$. But for $s \ll 1$ (which is like disorder), the $\langle E\rangle_r$ are different, implying non-uniform p_n distribution with $T_\infty < \infty$. This picture is confirmed by the numerical analysis.

Applications.– There are several proposed experiments that concern "sparse" systems. The most promising direction is the study of the heating rate of cold atoms in traps with vibrating walls [17], where the sparsity of the perturbation matrix is controlled either by the degree of chaoticity or by the strength of the inter-atomic interactions. In the condensed matter context, proposed experiments concern the rate of heating of small metallic particles by low frequency irradiation [15] (where the sparsity is due to the level spacing statistics), and the mesoscopic conductance of ballistic rings [15] (where the sparsity is due to the localization of the eigenstates in mode space), analogous to variable-range-hopping (where the sparsity is due to the Anderson localization) [18].

Discussion.– It is important to realize a common theme in the SLRT line of study and in the studies of FDT violation in glassy systems [12]. In both cases, we have to distinguish between "microscopic" and "macroscopic" time scales, and between "microscopic" and "macroscopic" temperatures. Eq.(2) and Eq.(3) establish a diffusion-dissipation relation involving a macroscopic temperature T that might be much lower compared with the microscopic temperatures T_n. The diffusion is driven by the fluctuations of the sources, but it is not the Kubo formula which should be used in order to determine D, but rather a resistor network SLRT calculation.

A closely related chain of works regarding NESS, concerns mixed phase-space of periodically driven systems [4–7], where the problem is reduced to the study of a stochastic rate equation. Our work differs in three respects: (1) The sparsity may arise even for quantized chaotic non-mixed systems, implying a glassy type of NESS; (2) We assume a stationary low frequency driving source rather than strictly periodic driving; (3) The master equation approach has allowed us to consider novel mesoscopic circumstances in which the quantum NESS differs enormously from the stochastic prediction.

The influence of quantum coherence on the NESS is remarkable. Taking into account the localization of the eigenstates in energy space, we found that for strong driving the temperature saturates to a *finite* value that reflects the sparsity of system. This should be contrasted with the traditional stochastic prediction of unbounded temperature.

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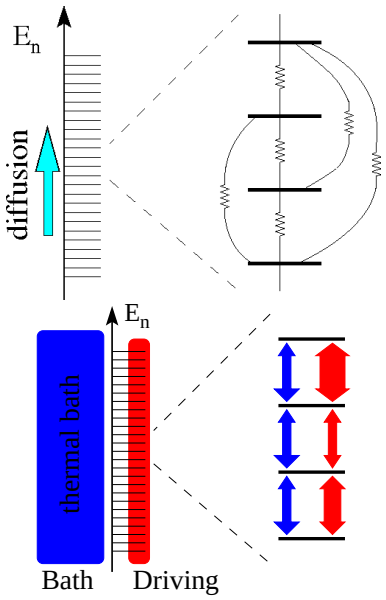

FIG. 1: Illustration of the model system. In the absence of a bath (upper panel) the driving induces transitions between levels E_n of a closed system, leading to diffusion in energy space and, hence, heating up of the system. The diffusion coefficient D can be calculated using a resistor network analogy. Connected sequences of transitions are essential in order to have a non-vanishing result, as in the theory of percolation. In the presence of a heat bath (lower panel) a NESS is reached: blue arrows represent the bath induced transitions (the bath favors downward transitions), while red arrows are the driving induced transitions (equal up-down transitions).

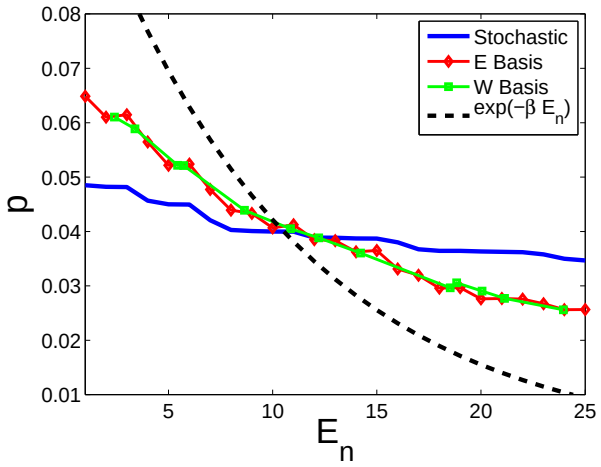

FIG. 2: The NESS occupation probabilities p_n are plotted vs E_n in the stochastic (blue) and quantum (red) cases. In the latter (quantum) case we plot also the occupation probabilities p_r of the W eigenstates versus $\langle E\rangle_r$. The sparsity is $s = e^{-5}$, and $\epsilon = 1000$. We observe that the effective temperature predicted by the quantum master equation is lower compared with the stochastic approximation.

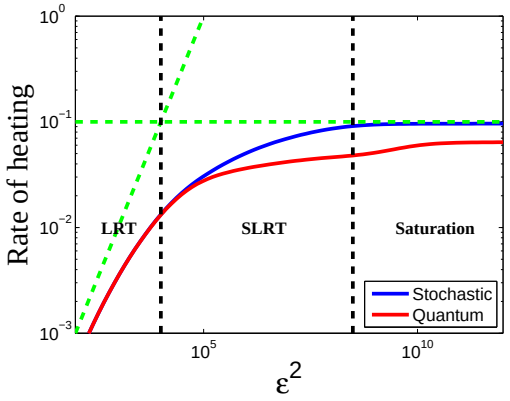

FIG. 3: The NESS heating rate $\dot{W}$ is calculated from the stochastic (blue) and quantum (red) master equations. The sparsity is $s = e^{-15}$. The vertical lines are plotted at values of ϵ for which the stochastic picture predicts a crossover.

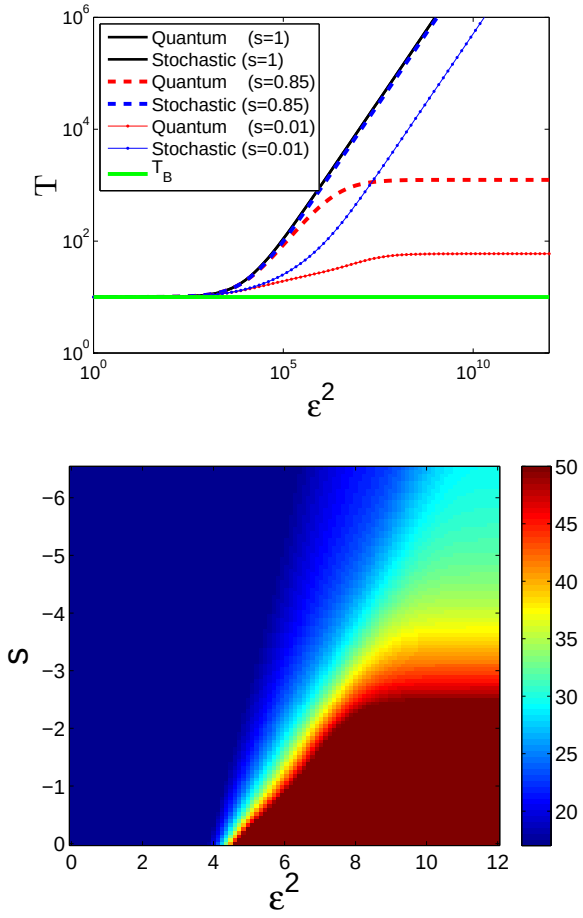

FIG. 4: The effective temperature T of the NESS is plotted versus the driving intensity (upper panel). Blue lines are for the stochastic NESS, while red lines are for the quantum NESS. The green line represents the temperature T_B of the bath. In the quantum case the effective temperature is imaged for additional values of the sparsity (lower panel). The color scale is limited for display purposes, and the axes are in log scale, i.e. $\log(\epsilon^2)$ and $\log(s)$.

SUPPLEMENTARY MATERIAL

Here we present the straightforward derivation that leads to the LRT/SLRT phenomenology.

The energy of the system is $E = \sum_n p_n E_n$, and its rate of change is $\dot{E} = \sum_n E_n \dot{p}_n$. The equation for $\dot{p}_n$ includes a driving source term and a bath term. Accordingly we write $\dot{E} = \dot{W} - \dot{Q}$, where the two terms are interpreted as the rate of heating due to the driving, and the rate of cooling due to the bath. From the master equation it follows that the expression for $\dot{Q}$ is

$$\dot{Q} = -\sum_{n,m}(E_n - E_m)\mathcal{W}^{\beta}_{nm}p_m \tag{16}$$

This expression can be written as the sum of a term that originates from the asymmetry of $\mathcal{W}^{\beta}_{nm}$, and a term that originates from the non-uniformity of the p_n. Defining $\bar{p}_{nm} = (p_n + p_m)/2$ we have

$$p_n - p_m = \left[2\tanh\left(-\frac{E_n - E_m}{2T_{nm}}\right)\right]\bar{p}_{nm} \tag{17}$$

$$\mathcal{W}^{\beta}_{nm} - \mathcal{W}^{\beta}_{mn} = \left[2\sinh\left(-\frac{E_n - E_m}{2T_B}\right)\right]w^{\beta}_{nm} \tag{18}$$

At high temperatures one can approximate the tanh() and the sinh() by linear functions leading to

$$\dot{Q} = \frac{1}{2}\sum_{n,m}\bar{p}_{nm}\frac{w^{\beta}_{nm}}{T_B}(E_n - E_m)^2 \tag{19}$$

$$- \frac{1}{2}\sum_{n,m}\bar{p}_{nm}\frac{w^{\beta}_{nm}}{T_{nm}}(E_n - E_m)^2 \tag{20}$$

The first expression is identified as D_B/T_B, where D_B is the bath induced diffusion coefficient. The second expression is used to define the effective temperature T, such that it takes the form $-D_B/T$.

In the *stochastic* case the effect of the driving can be treated using the same procedure. In analogy to Eq.(16) one can write

$$\dot{W} = \sum_{n,m}(E_n - E_m)w_{nm}p_m \tag{21}$$

Taking into account that w_{nm} is a symmetric matrix one obtains, in analogy to Eq.(20),

$$\dot{W} = \frac{1}{2}\sum_{n,m}\bar{p}_{nm}\frac{w_{nm}}{T_{nm}}(E_n - E_m)^2 \tag{22}$$

If the state is strictly canonical with all the T_{nm} equal the same number T, then $\dot{W} = D/T$ where

$$D_{[\mathrm{LRT}]} = \frac{1}{2}\overline{\sum_n w_{nm}(E_n - E_m)^2} \tag{23}$$

where the overline indicates canonical averaging over the initial state. This is the standard expression for the diffusion coefficient, leading to Eq.(4) in the case of near-neighbor transitions.

More generally T is the effective temperature, and the equation $\dot{W} = D/T$ is used to *define* the effective coefficient D. In the stochastic case Eq.(22) applies, and for near-neighbor transitions one obtains Eq.(5), which is like adding connectors in series. More generally, if we have a stochastic model, Eq.(22) implies that D can be found via a resistor network calculation [15].

We also attach below an additional figure.

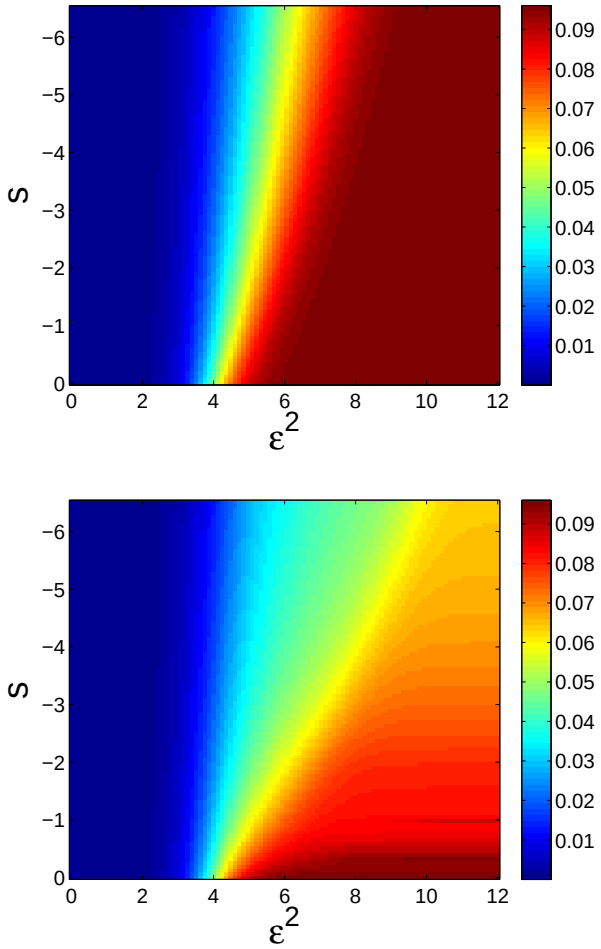

FIG. 5: Complementary to Fig. 3. The NESS heating rate $\dot{W}$ is calculated from the stochastic (upper) and quantum (lower) master equations. The quantum saturation value becomes lower as s becomes samller. The axes are in log scale.