

# Information and Entropy in Quantum Brownian Motion

## Thermodynamic Entropy versus von Neumann Entropy

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**Abstract** We compare the thermodynamic entropy of a quantum Brownian oscillator derived from the partition function of the subsystem with the von Neumann entropy of its reduced density matrix. At low temperatures we find deviations between these two entropies which are due to the fact that the Brownian particle and its environment are entangled. We give an explanation for these findings and point out that these deviations become important in cases where statements about the information capacity of the subsystem are associated with thermodynamic properties, as it is the case for the Landauer principle.

**Keywords** Quantum Brownian motion · Information · Entropy · Landauer principle

### 1 Introduction

Quantum systems that are not perfectly isolated from their environment are subject to dissipation and decoherence. Within the theory of quantum dissipative systems [7, 13, 37] models with system-reservoir interaction such as Quantum Brownian motion [11, 17] have been developed to describe these phenomena. The results are of great interest for applications in the field of mesoscopic systems, quantum computation [30] and quantum information theory of continuous variable systems [6, 12].

In last years the behavior of open quantum systems has also raised questions about the validity of fundamental laws of thermodynamics [4, 31, 35] and has again been addressed by recently published papers [18, 19, 23]. The central point in this discussion is the proper definition of the thermodynamic quantities of interest, especially the entropy. For this reason we want to provide a comprehensive overview of the two most common measures of the entropy of an open quantum system—the von Neumann entropy and the thermodynamic entropy—and point out that these two quantities might deviate in the quantum Brownian motion model.

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The entropy of a system in thermodynamic equilibrium was originally defined by Boltzmann as the logarithm of the number of microstates consistent with the properties of the macrostate—in quantum mechanics the logarithm of the dimension of the relevant Hilbert space. For a micro-canonical ensemble (where all the accessible microstates are equally likely) it is equivalent to the statistical entropy. The statistical entropy of a quantum system is given by the von Neumann entropy. The von Neumann entropy of a subsystem can be derived from the reduced density matrix [32]. In quantum information theory it is a commonly used measure of entanglement and decoherence [6] and can be understood as a measure of the amount of information gained by a unique quantum measurement of localization. The thermodynamic entropy, on the other hand, is associated with the amount of heat contained in the subsystem. Heat is defined as the part of the internal energy of a system which cannot be transferred into mechanical work. The thermodynamic entropy can be calculated from the partition function of the system and its free energy respectively.

As long as the application of the von Neumann entropy is restricted to an information-theoretical context and the thermodynamic entropy is applied when examining the validity of the thermodynamic laws no interpretational problems will arise. The situation is different in cases where statements about the information content of a system are connected to thermodynamic properties, as will be shown in the following.

This paper is organized as follows. In the first part of this paper we give a short review of the Caldeira-Leggett model of quantum Brownian motion which is the basis for discussion. In the main part the thermodynamic entropy and the von Neumann entropy are calculated and compared. Finally we discuss the significance of the deviations with regard to an information-theoretical point of view, namely by means of the Landauer principle.

## 2 Caldeira-Leggett Model of Quantum Brownian Motion

The statistical properties of the stationary state are discussed here on the basis of the Caldeira-Leggett model [9–11] of quantum Brownian motion, often referred to as independent oscillator model [15, 16]. It is a system-plus-reservoir model where the total Hamiltonian consists of three parts

$$H = H_s + H_b + H_{\text{int}}, \quad (1)$$

with  $H_s$  as Hamiltonian of the subsystem which interacts via the Hamiltonian  $H_{\text{int}}$  with a bath that is described by a collection of a large number  $N$  of harmonic oscillators  $H_b = \sum_i \hbar\omega_i (b_i^\dagger b_i + 1)$ . In detail the Hamiltonian of the Caldeira Leggett model is given by

$$H = \frac{p^2}{2m} + V(q) + \sum_{i=1}^N \left[ \frac{p_i^2}{2m_i} + \frac{m_i\omega_i^2}{2} \left( x_i - \frac{c_i q}{m_i\omega_i^2} \right)^2 \right], \quad (2)$$

where  $q$  and  $p$  are the Heisenberg-operators of coordinate and momentum of the Brownian oscillator moving in an harmonic potential  $V(q) = \frac{1}{2}m\omega_0^2 q^2$  and coupled to a bath of  $N$  independent harmonic oscillators with variables  $x_i$ ,  $p_i$  and equidistant frequencies  $\omega_i = i\Delta$ . The bath is characterized by its spectral density

$$J(\omega) = \pi \sum_{i=1}^N \frac{c_i^2}{2m\omega_i} \delta(\omega - \omega_i) = \frac{\gamma\omega\Gamma^2}{\omega^2 + \Gamma^2} \quad (3)$$

with cut-off frequency  $\Gamma = N\Delta$  and system-bath coupling strength  $\gamma$ . The interaction is bilinear in the coordinates  $q$  and  $x_i$  of the subsystem and the bath respectively with coupling parameters  $c_i = \sqrt{2\Delta m_i \omega_i J(\omega_i)/\pi}$ . The self-interaction term (proportional to  $q^2$ ) in the Hamiltonian

$$H_{\text{int}} = \sum_{i=1}^N \left[ -c_i x_i q + \frac{c_i^2}{2m_i \omega_i^2} q^2 \right] \tag{4}$$

renormalizes the oscillator potential to ensure that the observable frequency is close to bare oscillator frequency  $\omega_0$ . From the Hamiltonian (2) the Heisenberg equations of motion for the operators  $q$  and  $p$  and the bath variables  $x_i, p_i$  are received. By eliminating the bath degrees of freedom the quantum Langevin equation [14, 17] of a particle moving in the potential  $V(q)$  can be derived:

$$m\ddot{q}(t) + \frac{dV(q)}{dq} + \int_0^t dt' \gamma(t-t')\dot{q}(t') = \eta(t) - q(0)\gamma(t), \tag{5}$$

with damping kernel

$$\gamma(t) = \frac{2}{\pi} \int_0^\infty d\omega \frac{J(\omega)}{\omega} \cos \omega t = \gamma \Gamma e^{-\Gamma t} \tag{6}$$

and the noise term  $\eta(t)$  characterized by its correlation function [20]

$$K(t-t') = \frac{\hbar}{\pi} \int_0^\infty d\omega J(\omega) \coth\left(\frac{1}{2}\beta\hbar\omega\right) \cos \omega(t-t'). \tag{7}$$

The stationary state of the Brownian particle is fully characterized the reduced density matrix  $\rho_s$  of the subsystem [22, 37]

$$\langle q | \rho_s | q' \rangle = \frac{1}{\sqrt{2\pi \langle q^2 \rangle}} \exp \left[ -\frac{(q+q')^2}{8\langle q^2 \rangle} - \frac{(q-q')^2}{2\hbar^2/\langle p^2 \rangle} \right], \tag{8}$$

where the equilibrium fluctuations  $\langle q^2 \rangle, \langle p^2 \rangle$  and the susceptibility  $\tilde{\chi}(\omega) = [m\omega_0^2 - m\omega^2 - i\omega\tilde{\gamma}(\omega)]^{-1}$  with  $\tilde{\gamma}(\omega) = \int_0^\infty \gamma(t)e^{i\omega t}$  are connected by the quantum fluctuation-dissipation-theorem which gives

$$\langle q^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \coth\left(\frac{1}{2}\beta\hbar\omega\right) \text{Im}\{\tilde{\chi}(\omega)\}, \tag{9}$$

$$\langle p^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega m^2 \omega^2 \coth\left(\frac{1}{2}\beta\hbar\omega\right) \text{Im}\{\tilde{\chi}(\omega)\} \tag{10}$$

for the stationary correlations.

### 3 Calculation of Entropies

#### 3.1 Partition Function and Thermodynamic Entropy

Starting point in the calculation of thermodynamic quantities is the partition function. For dissipative quantum systems such as the QBM model it can be derived by influence func-

tional path integral methods [21],

$$\mathcal{Z} = \oint \mathcal{D}[q(t)] e^{-S_{\text{eff}}^E[q(t)]/\hbar} \tag{11}$$

with effective Euclidean action  $S_{\text{eff}}^E[q(t)]$  and is given by

$$\mathcal{Z} = \frac{1}{\beta \hbar \omega_0} \prod_{n=1}^{\infty} \frac{v_n^2}{\omega_0^2 + v_n^2 + v_n \hat{\gamma}(v_n)}, \tag{12}$$

with Laplace transform  $\hat{\gamma}(z)$  of (6) and Matsubara frequencies  $v_n = 2\pi n/\hbar\beta$ ,  $n = \pm 1, \pm 2, \dots$ . For the Drude model (3) the partition function can be rewritten in the form

$$\mathcal{Z} = \frac{\omega_0}{2\pi v} \frac{\Gamma_e(\lambda_1/v)\Gamma_e(\lambda_2/v)\Gamma_e(\lambda_3/v)}{\Gamma_e(\Gamma/v)}, \tag{13}$$

with the varGamma function  $\Gamma_e(x)$ ,  $v = |v_1|$  and  $\lambda_j$ ,  $j = 1, \dots, 3$  as three characteristic frequencies (poles) of the non-Markovian damped harmonic oscillator. The free energy

$$F = -kT \ln \mathcal{Z} = kT \left[ \ln \frac{\Gamma_e(\Gamma/v)}{\omega_0/(2\pi v)} - \sum_{j=1}^3 \ln \Gamma_e(\lambda_j/v) \right] \tag{14}$$

can also be written in the form [16, 19]

$$F(T) = \frac{1}{\pi} \int_0^{\infty} d\omega f(\omega, T) \text{Im} \left\{ \frac{d \ln \tilde{\chi}(\omega)}{d\omega} \right\}, \tag{15}$$

with  $f(\omega, T) = kT \ln[2 \sinh(\frac{1}{2}\beta\hbar\omega)]$  as free energy of the uncoupled harmonic oscillator. The thermodynamic entropy

$$S(T) = -\frac{\partial F}{\partial T} = \frac{1}{\pi} \int_0^{\infty} d\omega s(\omega, T) \text{Im} \left\{ \frac{d \ln \tilde{\chi}(\omega)}{d\omega} \right\}, \tag{16}$$

with  $s(\omega, T) = \frac{\beta\hbar\omega}{e^{\beta\hbar\omega}-1} - \ln(1 - e^{-\beta\hbar\omega})$  as well as the internal energy  $U = F + TS = -\frac{\partial}{\partial\beta} \ln \mathcal{Z}$  and the specific heat  $C = T \frac{\partial S}{\partial T}$  can then be calculated straightforward. At zero bath temperature the entropy vanishes  $\lim_{T \rightarrow 0} S(T) = 0$  as required by the Third Law of thermodynamics [18, 23]. In case of an ohmic heat bath, the entropy vanishes linearly with  $T$ . A interpretation of the free energy (15) will be given in section V within the discussion on cyclic thermodynamic processes.

### 3.2 Ground State Energetics at Zero Temperature

Despite the fact that the entropy (16) vanishes for  $T \rightarrow 0$  the energy of the subsystem fluctuates. Considering the subsystems Hamiltonian  $H_s$  as an observable of interest, projective measurements of  $H_s$  can find the system in higher energy states even at zero temperature [8, 25]. This is the case when subsystem and environment are entangled and therefore the ground state does not factorize into a product of a system wave function and a bath wave function. Formally it is a consequence of the fact that the Hamiltonian  $H_s$  does not commute

with the Hamiltonian  $H$  of the total system. The mean energy of an oscillator coupled to a heat bath which is given by the expression

$$\begin{aligned} \langle H_s \rangle &= \text{Tr}[\rho_s H_s] = \frac{1}{2m} \langle p^2 \rangle + \frac{1}{2} m \omega_0^2 \langle q^2 \rangle \\ &= \frac{m\hbar}{2\pi} \int_0^\infty d\omega (\omega_0^2 + \omega^2) \coth\left(\frac{1}{2}\beta\hbar\omega\right) \text{Im}\{\tilde{\chi}(\omega)\} \end{aligned} \tag{17}$$

is greater than its ground state energy for  $T \rightarrow 0$ :

$$\langle H_s \rangle_{T=0} = \frac{m\hbar}{2\pi} \int_0^\infty d\omega (\omega_0^2 + \omega^2) \text{Im}\{\chi(\omega)\} > \frac{1}{2}\hbar\omega_0. \tag{18}$$

The probability to measure the harmonic oscillator in the ground state or an excited state may be found by considering the diagonal matrix elements  $\rho_{nn}$  of the density matrix  $\rho_s$  in the energy basis

$$\rho_{nm} = \langle n | \rho_s | m \rangle = \int dq dq' \langle n | q \rangle \langle q | \rho_s | q' \rangle \langle q' | m \rangle, \tag{19}$$

where  $\langle q | n \rangle = (\sqrt{\pi} 2^n n!)^{-1/2} \sqrt{b} H_n(bq) e^{-b^2 q^2/2}$  are the wave functions of the harmonic oscillator with Hermite polynomials  $H_n$  and  $b = \sqrt{m\omega_0/\hbar}$ . The diagonal elements can then be expressed explicitly by

$$\rho_{nn} = \sqrt{\frac{4}{D}} (d^2 - a^2)^{n/2} P_n \left[ \frac{d}{\sqrt{d^2 - a^2}} \right], \tag{20}$$

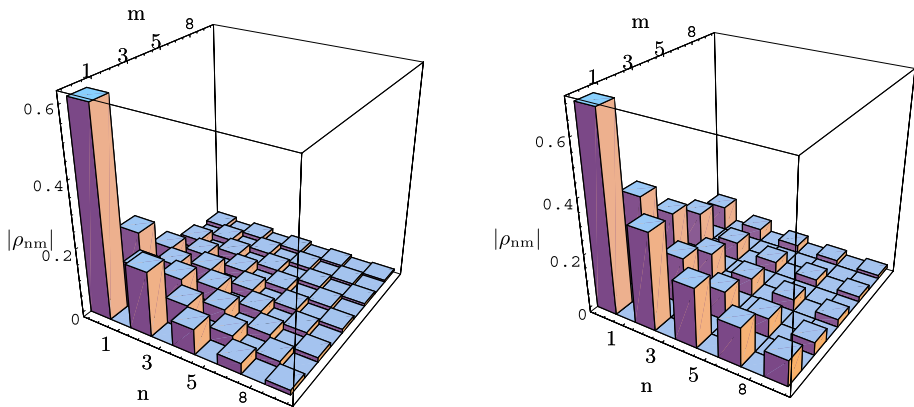
where  $P_n$  are the Legendre polynomials of order  $n$  and the dimensionless variables  $x = 2b^2 \langle q^2 \rangle$ ,  $y = 2\langle p^2 \rangle / (\hbar^2 b^2)$ ,  $D = 1 + x + y + xy$ ,  $a = (y - x) / D$  and  $d = (xy - 1) / D$  have been introduced [25]. As can be seen from Fig. 1a the density matrix  $\rho_{nm}$  is not strictly diagonal in this basis because the wave functions of the unperturbed oscillator are not the eigenfunctions of  $\rho_s$ . Furthermore, the eigenvalues  $p_n$  of  $\rho_s(q, q')$  and its eigenfunctions  $f_n = (\sqrt{\pi} 2^n n!)^{-1/2} \sqrt{c} H_n(cq) e^{-c^2 q^2/2}$  with  $c = [\langle p^2 \rangle / (\hbar^2 \langle q^2 \rangle)]^{1/4}$  are obtained as solution of the problem  $\int dq' \rho(q, q') f_n(q') = p_n f_n(q)$  [4]. Making use of the purity

$$\mu = \text{Tr} \rho_s^2 = \int dq dq' \langle q | \rho_s | q' \rangle \langle q' | \rho_s | q \rangle = \frac{\hbar/2}{\sqrt{\langle q^2 \rangle \langle p^2 \rangle}} \tag{21}$$

the eigenvalues can be expressed by

$$p_n = 2\mu / (1 + \mu) \left[ (1 - \mu) / (1 + \mu) \right]^n. \tag{22}$$

Figure 1a visualizes the distribution of the density matrix elements in the energy eigenbasis of the QBM-state at low temperatures. One can see that the density matrix in energy eigenbasis is not strictly diagonal and that the distribution on the diagonal deviates from the Boltzmann distribution. This is due to the interaction which correlates system and environment and additionally leads to a squeezed-like state. This becomes obvious when comparing Fig. 1a to Fig. 1b which shows the distribution of a squeezed vacuum state. Unlike the squeezed vacuum state, the stationary QBM-state is not a pure state with minimal uncertainty but a mixed state even at zero bath temperature. Diagonalizing the density matrix (8)



(a) Density matrix elements  $\rho_{nm}$  of the stationary QBM-state given by equation (19) for mean occupation number  $\langle n \rangle = 1$  ( $\Gamma = 100\omega_0$ ,  $\gamma \approx 2\omega_0$ ) at low bath temperature  $T = 10^{-3}\hbar\omega_0/k$ . The stationary QBM-state is a mixed state with purity  $\mu < 1$ .

(b) Density matrix elements  $\rho_{nm}$  of a squeezed vacuum state  $|\xi\rangle$  with mean occupation number  $\langle n \rangle = \sinh^2|\xi| = 1$ . The squeezed vacuum state is a pure state with purity  $\mu = 1$ .

**Fig. 1** (Color online) Density matrix elements  $\rho_{nm}$  of the stationary QBM-state (left) compared to the density matrix elements of a squeezed vacuum state  $|\xi\rangle = e^{\xi^*a^2/2 - \xi(a^\dagger)^2/2}|0\rangle$  (right) with equal mean occupation number  $\langle n \rangle$

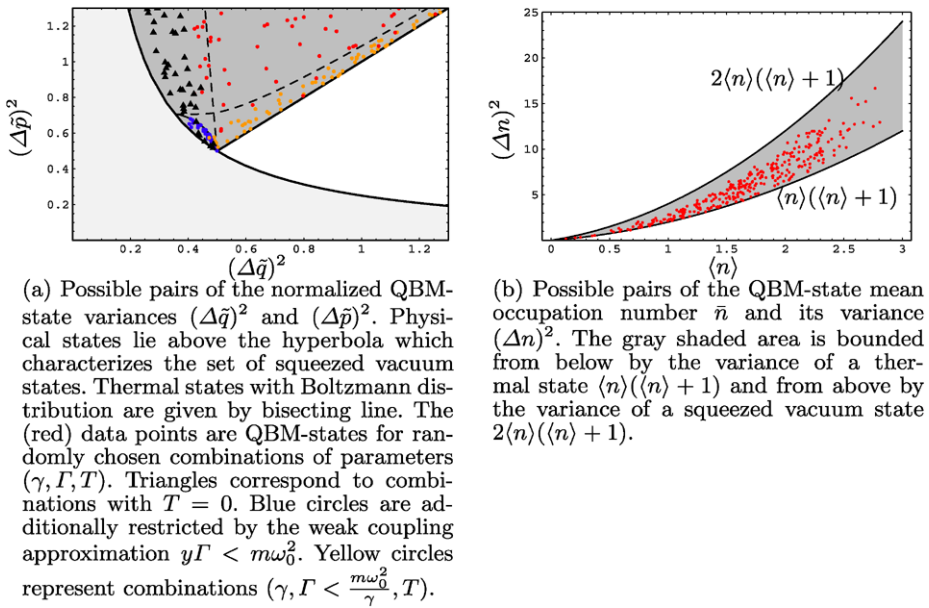
does not just yield one eigenvalue unequal to zero ( $p_0 = 1$ ,  $p_n = 0$  for  $n > 0$ ), but also  $p_n > 0$  for  $n > 0$ . Thus, for non-weak system bath interaction with  $\gamma > 0$  and zero temperature the purity is  $\mu < 1$  and the von Neumann entropy  $S_v(\rho_s) > 0$ . Despite the same occupation number  $\langle n \rangle$  in Figs. 1a and 1b, the purity and the von Neumann entropy are different in both cases.

The environment-induced squeezing increases the uncertainty product  $\Delta q \Delta p$  compared to a thermal state. This can be seen from Fig. 2a which shows possible and feasible combinations of the second moments of  $p$  and  $q$ . Physical states lie above the hyperbola which characterizes the set of squeezed vacuum states. Thermal states with Boltzmann distribution are given by the bisecting line. The data points in the gray shades area are QBM-states for randomly chosen combinations of parameters  $(\gamma, \Gamma, T)$ . Possible pairs of the mean occupation number  $\bar{n}$  and its variance  $(\Delta n)^2$  for arbitrary combinations of  $\gamma, \Gamma$  and  $T$  in the QBM model are bounded from below by the variance of a thermal state  $\langle n \rangle(\langle n \rangle + 1)$  and from above by the variance of a squeezed vacuum state  $2\langle n \rangle(\langle n \rangle + 1)$ . This is illustrated by Fig. 2b.

The statistical properties of the stationary QBM-state hence are a consequence of the thermal noise, environment-induced squeezing and existing quantum correlations between system and bath. The distribution of the diagonal elements in the energy eigenbasis thus deviates from the Boltzmann distribution. Figure 3 visualizes the difference between (22) and  $\rho_{nn}$  evaluated in (19). The population of higher levels is increased while the population of lower levels is reduced compared to a thermal distribution.

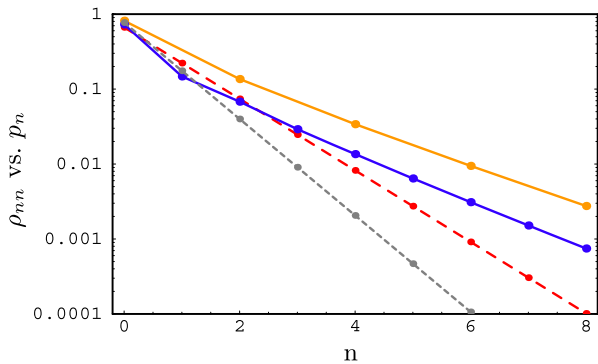
### 3.3 Reduced Density Matrix and von Neumann Entropy

Since the probability to find the system in an excited state does not vanish even at zero temperature, the density operator  $\rho_s$  does not reduce to the projection onto the non-degenerate



**Fig. 2** (Color online) *Left*: Possible pairs of the normalized QBM-state variances  $(\Delta\tilde{q})^2 = (\Delta q)^2/\sigma_0$  and  $(\Delta\tilde{p})^2 = (\Delta p)^2 4\sigma_0^2/\hbar^2$ . *Right*: Possible pairs of the QBM-state mean occupation number  $\bar{n}$  and its variance  $(\Delta n)^2$

**Fig. 3** (Color online) Distribution of the diagonal density matrix elements  $\rho_{nn}$  of a QBM-state with  $\langle n \rangle = 1/2$  (blue line) compared to a squeezed vacuum state (yellow line) and a thermal state (red line) with the same occupation number (on a logarithmic scale). The distribution of the eigenvalues  $p_n$  given by (22) is the dashed gray line ( $\Gamma = 100\omega_0, \gamma = 0.93\omega_0$ )



ground state of the system  $H_s$  and thus does not describe a pure state with statistical entropy equal to zero. The uncertainty about the measurement outcome is expressed by the von Neumann entropy  $S_v(\rho_s)$  of the reduced density matrix  $\rho_s$  which is in the case of a Gaussian state given by [1, 4, 34]:

$$S_v(\rho_s) = -k \text{Tr}[\rho_s \ln \rho_s] = -k \sum_n p_n \ln p_n = k \frac{1-\mu}{2\mu} \ln \frac{1+\mu}{1-\mu} - k \ln \frac{2\mu}{1+\mu}.$$

Introducing the effective frequency and mass [37]

$$\omega_{\text{eff}} = \frac{2}{\hbar\beta} \operatorname{arccoth}(\mu), \quad m_{\text{eff}} = \frac{\sqrt{\langle p^2 \rangle / \langle q^2 \rangle}}{\omega_{\text{eff}}}, \quad (23)$$

the density matrix can be written in the form

$$\rho_s = Z_{\text{eff}}^{-1} \exp(-\beta H_{\text{eff}}), \quad (24)$$

with effective partition function  $Z_{\text{eff}}^{-1} = 2 \sinh(\omega_{\text{eff}} \hbar \beta / 2)$  and Hamiltonian  $H_{\text{eff}} = \frac{p^2}{2m_{\text{eff}}} + \frac{1}{2} m_{\text{eff}} \omega_{\text{eff}}^2 q^2$ . The von Neumann entropy and its eigenvalues  $p_n$  can then be expressed by

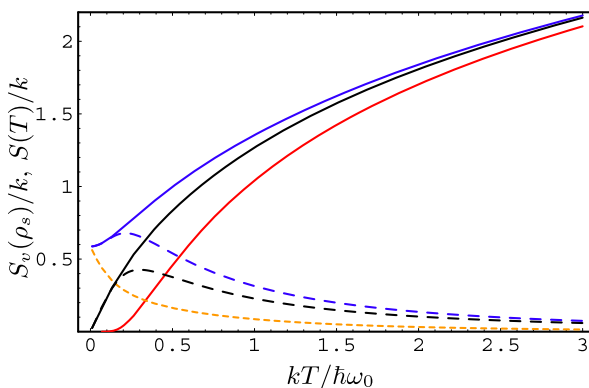
$$S_v(\rho_s) = \frac{\beta \hbar \omega_{\text{eff}}}{e^{\beta \hbar \omega_{\text{eff}}} - 1} - \ln(1 - e^{-\beta \hbar \omega_{\text{eff}}}), \quad (25)$$

and  $p_n = Z_{\text{eff}}^{-1} e^{-\beta E_n}$  with  $E_n = \hbar \omega_{\text{eff}}(n + 1/2)$ . However, notice that  $S_v(\rho_s) \neq S_{\text{eff}} = \frac{\partial}{\partial T}(kT \ln Z_{\text{eff}})$  due to the temperature dependence of  $\omega_{\text{eff}}$ . Since  $\omega_{\text{eff}} \rightarrow 0$  for  $T \rightarrow 0$  the effective energy levels  $E_n$  become very narrowly spaced near zero temperature indicating that the ground state is a mixture.  $S_v(\rho_s)$  is the minimal amount of classical information that is accessible through measurements on the quantum state  $\rho_s$  [30] and is thus smaller than the Shannon entropy  $\sum_n \rho_{nn} \log \rho_{nn}$  with matrix elements  $\rho_{nn}$  given in the basis of the unperturbed eigenfunctions of the harmonic oscillator (which are not the eigenfunctions of  $\rho_s$ ).

### 4 Comparison of Entropies

The von Neumann entropy  $S_v$  of the subsystem  $\rho_s$  and the thermodynamic entropy  $S(T)$  of the Brownian particle deviate from each other as one can see from Fig. 4:

$$S_v(\rho_s) \geq S(T) \quad \text{for } \gamma > 0. \quad (26)$$



**Fig. 4** (Color online) Temperature dependence of the von Neumann entropy  $S_v(\rho_s)$  (blue line), thermodynamic entropy  $S(T)$  (dark line) and function  $s(\omega, T)$  (red line) for system-bath-coupling  $\gamma = 10m\omega_0^2/\Gamma = 1$  compared to the entropy of the uncoupled harmonic oscillator  $s(\omega, T)$  (dashed lines for the corresponding differences  $S_v(\rho_s) - s(\omega, T)$  (blue),  $S(T) - s(\omega, T)$  (black) and  $S_v(\rho_s) - S(T)$  (yellow)). Parameters are  $\Gamma = 10\omega_0$  and  $\gamma \approx 2.43\omega_0$ , thus having  $(H_s)_{T=0} = \hbar\omega_0$



Even at  $T \rightarrow 0$  the von Neumann entropy  $S_v$  is larger than zero while its thermodynamic entropy vanishes approximately linearly with  $T$ . This effect of  $S_{v,T \rightarrow 0} \neq 0$  which has been extensively discussed in Refs. [3, 4] is due to the entanglement between subsystem and bath which prevents the subsystem from reaching a pure state for  $T = 0$ . It is just in the weak coupling limit  $\gamma \rightarrow 0$  that the von Neumann entropy (23) and the thermodynamic entropy (16) become equal and tend towards the entropy  $s(\omega_0, T)$  of a harmonic oscillator in a heat bath at temperature  $T$ , characterized by the Gibbs distribution.

The reason for the deviation in entropies may be seen in the fact that the density matrix  $\rho_s$  cannot be written in canonical form

$$\rho_s \neq \frac{1}{Z} \exp(-\beta H_s). \tag{27}$$

The statistical entropy can be identified with the thermodynamic entropy just if  $\rho = Z^{-1} \exp(-\beta H_s)$  is the canonical density matrix with  $Z = \text{Tr}[\exp(-\beta H_s)]$ , which means

$$\begin{aligned} S_v(\rho) &= -\text{Tr}[\rho \ln \rho] = \beta \text{Tr}[\rho H_s] + \text{Tr}[\rho \ln Z] = \beta \langle H_s \rangle + \ln Z \\ &= \beta(U - F) = S(T). \end{aligned} \tag{28}$$

In the same manner, the heat  $\delta Q$  connected to the thermodynamic entropy by the Clausius equality  $\delta Q = T dS$  (for quasi-static processes) can only be associated with the part of  $dU$  representing a statistical redistribution in phase space  $\text{Tr}[d\rho_s H_s]$  if  $\rho_s$  is given in canonical form:

$$dS_v = -\text{Tr}[d\rho \ln \rho] = \text{Tr}[d\rho \ln Z] + \beta \text{Tr}[d\rho H_s] = \beta \text{Tr}[d\rho H_s] = \beta \delta Q = dS(T). \tag{29}$$

While the choice of the entropy (16) implies that this thermodynamic entropy of the Brownian oscillator  $S(T)$  and the (unperturbed) bath  $S_v(\rho_b)$  are additive—since all correlations between bath and oscillator are included in the subsystems entropy—the von Neumann entropy (23) for the system and the bath entropy are non-additive

$$S_v(\rho_s) + S_v(\rho_b) - I_{sb} = S_v(\rho_{\text{tot}}) = S(T) + S_v(\rho_b), \tag{30}$$

with non-zero mutual information/entropy  $I_{sb}$  measuring the correlations between the parts  $S$  and  $B$  of the entangled system  $\rho_{\text{tot}} \neq \rho_s \otimes \rho_b$ . The conditional entropy  $S(S|B) = S_v(\rho_s) - I_{sb}$  can be identified with the thermodynamic entropy (16). This entropy measures the uncertainty about the state of  $S$  if the state of  $B$  is known [30]. It is the shift in the total von Neumann entropy  $S_v(\rho_{\text{tot}}) - S_v(\rho_b)$  due to the presence of the Brownian particle and thus differs strongly from the von Neumann entropy  $S_v(\rho_s)$  of the particle alone.

### 5 Cyclic Thermodynamic Processes

The theoretical result of a mean energy  $\langle H_s \rangle_{T \rightarrow 0} > \frac{1}{2} \hbar \omega_0$  has raised the question whether this is a contradiction to the second law: if the particle is subtracted from the bath the difference in energy could be used to perform work. A cyclic process could be constructed that receives energy for work generation from a single heat bath. That such a construction of a perpetuum mobile of the second kind is not possible was recently shown by Ford and O’Connell [19] for the QBM-model with Lorentzian bath spectral density and by Kim and Mahler [26] for arbitrary bath spectra. The basic argument is the principle of minimal work

which states that the minimal amount of work that is needed to bring the system from one thermodynamic state to another of the same temperature, is equal to the difference in the free energy of these two thermodynamic states [27]. If the Brownian oscillator is added to or subtracted from the bath the difference in free energy is equal to  $F(T)$  in (14). This can be seen from the following considerations. The free energy of the total system is given by the sum

$$F_{\text{tot}}(T, \gamma) = \sum_k f(\omega'_k, T), \tag{31}$$

where the eigenfrequencies  $\omega'_k$  of the coupled system follow as the roots of a transcendental eigenvalue equation [4] and  $f(\omega'_k, T) = kT \ln 2 \sinh(\frac{1}{2}\beta\hbar\omega'_k)$ . For  $\omega_k \gg \Delta$  the initial frequencies  $\omega_k = k\Delta$  get shifted to

$$\omega'_k = \omega_k - \frac{\Delta}{\pi} \phi(\omega_k) \quad \text{for } \omega_k \gg \Delta, \tag{32}$$

where  $\phi(\omega)$  is related to the susceptibility  $\tilde{\chi}(\omega)$  by

$$\phi(\omega) = \int_0^\omega dv \operatorname{Im} \left\{ \frac{d \ln \tilde{\chi}(v)}{dv} \right\} = \sum_{j=1}^3 \arctan \frac{\omega}{\lambda_j} - \arctan \frac{\omega}{\Gamma}. \tag{33}$$

Using the identity (for small  $\Delta$ )

$$\sum_k f(\omega'_k) \rightarrow \frac{1}{\Delta} \int_0^\infty d\omega'_k \frac{d\omega_k}{d\omega'_k} f(\omega'_k), \tag{34}$$

the total free energy (31) can be written as

$$F_{\text{tot}}(T, \gamma) = \int_0^\infty d\omega \left[ \frac{1}{\Delta} + \frac{1}{\pi} \frac{d\phi(\omega)}{d\omega} \right] f(\omega, T) \tag{35}$$

$$= \sum_k f(\omega_k, T) + \frac{1}{\pi} \int_0^\infty d\omega f(\omega, T) \frac{d\phi(\omega)}{d\omega} \tag{36}$$

$$= F_b(T, \gamma = 0) + F(T), \tag{37}$$

where  $F_b(T, \gamma = 0)$  is the free energy of the undisturbed bath in absence of the particle. Thus, the shift in free energy due to the coupling of the central oscillator to the bath is  $F(T)$ . The related increase in internal energy is then expressed by  $U(T) = F(T) + TS(T)$ . However, the mean energy of the oscillator is given by (17). To ensure the validity of the second law at zero temperature, the work which has to be performed has to be larger than the mean energy. Because of  $F(0) - \langle H \rangle_{T=0} \geq 0$  this is the case [19, 26]. Since at  $T \rightarrow 0$  all the employed work is converted into internal energy  $U(0)$  of the total system, the difference can be interpreted as interaction energy  $U_{\text{int}}$  (which is different from  $\langle H_{\text{int}} \rangle$ !). Due to the infinite number of bath modes this increase in internal energy does not raise the bath temperature. The interaction energy is given by the partial differentiation of the free energy (14) with respect to the cut-off frequency [4]

$$U_{\text{int}} = U - \langle H_s \rangle = \Gamma \frac{\partial F}{\partial \Gamma}. \tag{38}$$

With these considerations the zero temperature behavior of the thermodynamic entropy becomes plausible. The free energy  $F(0)$  is completely converted into internal energy  $U(0)$ , that is  $\langle H_s \rangle$  and  $U_{\text{int}}$ . This increase in internal energy is not accompanied by a flow of heat or a change in entropy at zero temperature, thus  $S(0) = 0$  and  $S_v(\rho_{\text{tot}}) = S_v(\rho_b(0))$ . On the other hand, variations of the oscillator parameters  $d\omega_0, dm$  are related to a change in entropy  $dS(T)$  and a heat flow respectively that can be calculated by comparing the total differential

$$dU = d\langle H_s \rangle + dU_{\text{int}} = \text{Tr}[\rho_s dH_s] + \text{Tr}[H_s d\rho_s] + dU_{\text{int}} = \delta W_s + \delta Q_s + dU_{\text{int}} \quad (39)$$

with the total differential  $dU = dF + TdS$ . A short calculation reveals that  $dF = \delta W_s := \text{Tr}[\rho_s dH_s]$  and thus one has

$$\delta Q := TdS(T) = \delta Q_s + dU_{\text{int}}. \quad (40)$$

Defining the total heat flow  $\delta Q$  accompanying a variation of the entropy  $S(T)$  by the Clausius (in)equality  $\delta Q = TdS(T)$  it becomes clear that a change in the thermodynamic entropy of the Brownian oscillator does not just lead to a heat flow expressed by a redistribution in phase space of the subsystem  $\text{Tr}[H_s d\rho_s] =: \delta Q_s$  but also to a flow of heat to the cloud of surrounding bath modes which is  $\delta Q_s = -dU_{\text{int}}$  for  $T \rightarrow 0$ . For a recent discussion on problems arising from a definition of local heat and work in bipartite quantum systems see e.g. Ref. [36].

### 6 Consequences for Quantum Information Theory

From an information-theoretical point of view, these considerations become important if statements about the information capacity of a quantum system are connected to thermodynamic properties. We may cite the Landauer principle [5, 28] as an example here. This principle is based on the Clausius inequality and states that many-to-one-operations like erasure of information requires the dissipation of energy. Deleting one bit of information of the systems memory is accompanied by a released amount of heat of at least  $kT \ln 2$ :

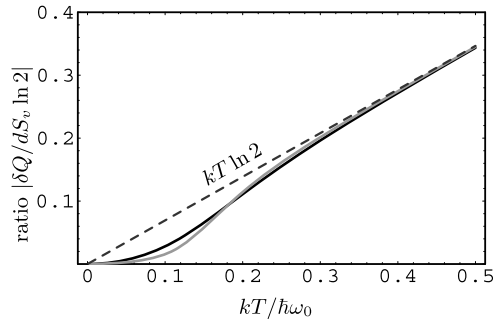
$$\left| \frac{\delta Q}{dS/(\ln 2)} \right| \geq kT \ln 2. \quad (41)$$

In our case we apply the Landauer principle to quantum systems in which classical information is encoded. Since the optimal erasure procedure, i.e. the one that creates the least amount of heat is the one where the quantum measurements are made in the basis of the eigenstates of  $\rho_s$ , the relevant entropy is the von Neumann entropy  $S_v(\rho_s)$  of the system. The erasure of information is connected to a reduction of entropy, and thus cannot be realized in a closed system. Therefore the information-carrying system has to be coupled to the environment. In a low temperature environment the coupling may be relatively strong compared to the thermal energy and system and bath become correlated.

Of course, the customary understanding of Landauer’s principle is that it applies to situations in which the information-bearing system is uncorrelated with the environment both initially and finally. Classically Landauer’s principle holds as long as the second law of thermodynamics is applicable in the given situation. With existing correlations between system and environment both principles—the Landauer bound as well as the second law—are not applicable because the basic requirement of additivity is not fulfilled. So, why considering the Landauer principle in this context? The point is, that in our case of quantum Brownian

**Fig. 5** (Color online)

Temperature dependence of the ratio  $|\delta Q/dS_v \ln 2|$  (in bits) with the heat defined by  $\delta Q = TdS(T)$  for quasi-static variations of the oscillator frequency  $d\omega_0$ . The system-bath-couplings are chosen to be  $\gamma = 0.1\omega_0$  (dark line) and  $\gamma = 0.5\omega_0$  (gray line). At low  $T$  deviations from the Landauer bound  $kT \ln 2$  (dashed line) occur. Here  $\Gamma = 10\omega_0$



motion the second law of thermodynamics holds as has been pointed out in the literature [18, 19, 23] while the Landauer principle may not be applicable as long as the von Neumann entropy of the reduced density matrix is seen as the relevant quantity to describe the classical information content of the quantum state of the damped harmonic oscillator. The reason for this is, that the von Neumann entropy and the thermodynamic entropy may deviate from each other for mesoscopic quantum systems that are sufficiently strong entangled with their environment. Since the statistical entropy and the heat are defined separately they do not necessarily have to fulfill the Clausius inequality [3, 24]. A second reason for considering the Landauer principle in this context is, that we are able to quantify the deviations from the Landauer bound that are resulting from the quantum correlations between the information carrying subsystem and its surrounding bath. At least it might be interesting to see in which way deviations from the Landauer principle occur if the assumption of weak interaction between system and bath is gradually abandoned.

As an example for our system we show in Fig. 5 the temperature dependence of the heat exchange  $\delta Q$  divided by the entropy change, in this case of the von Neumann entropy  $dS_v$  (in bits). The heat is defined by  $\delta Q = TdS(T)$  for quasi-static variations of the oscillator frequency  $d\omega_0$ . Since  $\delta Q_s$  and  $\delta Q_{\text{int}}$  can have different signs, the heat flow  $\delta Q$  is lowered compared to the term  $\delta Q_s$ . Thus, as it can clearly be seen, this ratio for small temperatures is *below* the Landauer bound of  $kT \ln 2$ . Actually at low temperature and high cut-off frequency this quantity starts out quadratically as a function of temperature instead of linearly, which is due to the fact that the von Neumann entropy term is larger than its canonical form (thermodynamic entropy) and therefore the Landauer principle in this case gives only an upper bound to the erasure of information.

## 7 Summary and Conclusions

In this paper we have studied the statistical and thermodynamic properties of the stationary QBM-state. We have shown that an identification of the thermodynamic entropy of the damped quantum oscillator with its von Neumann entropy is not valid except in the weak coupling limit. We have chosen Landauer's principle to determine these deviations qualitatively and quantitatively.

The statistical entropy associated with the stationary quantum state is the von Neumann entropy. The main features of the subsystem (e.g. mixed state at zero temperature, accessible information by measurements) are captured by the von Neumann entropy of the reduced density matrix. As a well established measure of entanglement and decoherence in open

quantum systems it is commonly in use—but interpretational problems may arise if it is related to thermodynamic quantities.

The thermodynamic entropy is the correct choice when cyclic processes are considered (e.g. to show that no work can be extracted from a single thermal bath [2, 19, 29, 33]). The exchange of heat between the system and the environment during quasi-static processes is related to the thermodynamic entropy by the Clausius (in)equality. However, it is misleading to speak of *the* entropy of the Brownian particle as we have pointed out. The thermodynamic entropy can just be identified with the statistical entropy when  $\rho_s$  takes the form of the canonical density matrix. This is just the case for negligible interaction between subsystem and environment. As long as the application of the von Neumann entropy is restricted to an information-theoretical context and the thermodynamic entropy is applied when examining the validity of the thermodynamic laws no interpretational problems will arise. The situation is different in cases where statements about the information content of a system are connected to thermodynamic properties as has been demonstrated by means of the Landauer principle. In this case the entanglement between the subsystem and the bath is responsible for the fact that the erasure of information—measured by the decrease in the von Neumann entropy of the reduced density matrix—is accompanied by a released amount of heat that may be below the Landauer bound.

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