THE QUANTUM LIMIT AT THERMAL EQUILIBRIUM

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1. Abstract

The aim of constructing and designing machines working at the nanometre-length scale has boosted the developing of a quantum version of thermodynamics. One of the foundational conundra in this emerging field is, to what extent nanomachines can display quantum features and how this quantum behaviour could be used to improve their efficiency. Intuitively, one can suggest that if the energy of the thermal fluctuations is much smaller than the typical energy scale of the nanosystem, then there is room for the nanosystem to revels its quantum nature. However, as it has been discussed recently in almost all fields related to quantum mechanics, the border between the quantum/classical operating regime is far from being trivial. We predict here, at thermodynamical equilibrium, the existence of a regime where, e.g., nanoelectromechanical structures or optomechanical systems can be found in an entangled state at high temperature assisted by the non-Markovian interactions. Our findings not only provides a solid ground for understanding the presence of quantum features in most of current investigations in bio and handmade systems, but also points out the direction to follow in protecting and isolating of quantum systems.

2. Canonical Typicality

From statistical mechanics, a physical system S coupled to a thermal bath B thermalizes into a state that is described by the canonical Boltzmann distribution. This is known as canonical typicality.

If the system S is described by the Hamiltonian $\hat{H}_{\mathrm{S}}$, the canonical distribution then reads

$$\hat{\rho}_{\mathrm{can}} = Z_{\mathrm{can}}^{-1} \exp(-\hat{H}_{\mathrm{S}}\beta),$$

where $Z_{\mathrm{can}} = \mathrm{tr}\{\exp(-\beta \hat{H}_{\mathrm{S}})\}$ denotes the partition function and $\beta = 1/k_{\mathrm{B}}T$ being T the temperature of the environment and k_{B} the Boltzmann constant.

If we characterize the bath by means of the Hamiltonian H_{B} and the interaction between the system and the bath by H_{SB}, then the equilibrium state of S is, in general, given by

$$\hat{\rho}_{\mathrm{S}} = Z^{-1} \mathrm{tr}_{\mathrm{B}} \exp\left[-\left(\hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{B}} + \hat{H}_{\mathrm{SB}}\right)\beta\right],$$

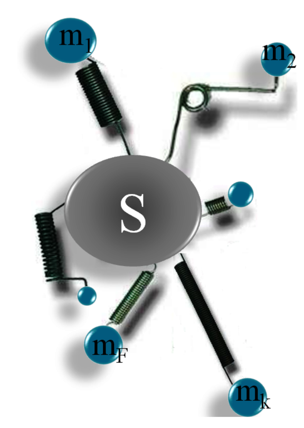
where Z is a *total* partition function [cf. Phys. Rev.Lett. 102, 210401 (2009)] given by $Z = \mathrm{tr}\, e^{-\beta(\hat{H}_{\mathrm{S}}+\hat{H}_{\mathrm{B}}+\hat{H}_{\mathrm{SB}})}$. This expression is valid for any coupling strength or temperature regime.

Deviations from canonical typicality imply that the system, at equilibrium, is described by a density density operator which is not diagonal in the eigenstates of H_{S}. In linear systems, such as quantum nano-mechanical resonators, this will imply the presence of squeezed steady states. However, one has to be careful at identifying this squeezing as a true quantum feature.

3. Model and Open quantum systems at equilibrium

We assume that the system B is composed of a collection of independent harmonic oscillators with masses m_j, frequencies ω_j and coupled linearly to S with constant couplings c_j. The total Hamiltonian $\hat{H} = \hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{B}} + \hat{H}_{\mathrm{SB}}$ can be explicitly written as

$$\hat{H} = \frac{\hat{p}^2}{2m_0} + \frac{m_0\omega_0^2}{2}\hat{q}^2 + \sum_j^{\infty} \frac{\hat{p}_j^2}{2m_j} + \frac{m_j\omega_j^2}{2}\left(\hat{q}_j - \frac{c_j}{m_j\omega_j^2}\hat{q}\right)^2.$$



The equilibrium matrix density of the bath is given by a path integral in imaginary time [Phys. Rep. 168, 115 (1988)]. When we consider the coupling, the density-matrix elements can be written as

$$\rho_\beta(q,q') = \frac{1}{\mathcal{Z}}\int \mathcal{D}q \exp\left(-\frac{1}{\hbar}S_{\mathrm{S}}^{\mathrm{E}}(q)\right)\mathcal{F}(q),$$

where the influence functional $\mathcal{F}(q)$ describes the influence of the environment on the system and it is given by

$$\mathcal{F}(q) = \exp\left(-\frac{1}{2\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\int_0^{\hbar\beta}\mathrm{d}\sigma k(\tau-\sigma)q(\tau)q(\sigma)\right),$$

where $k(\tau)$ is the kernel related to the Laplace transform of the damping kernel $\gamma(t)$, writing as

$$k(\tau) = \frac{m}{\hbar\beta}\sum_{l=-\infty}^{\infty}|\nu_l|\tilde{\gamma}(\nu_l)\exp(i\nu_l\tau),$$

where $\nu_l = 2\pi l/\hbar\beta$ are the Matsubara frequencies. The thermal bath is described by means of the most commonly used spectral density, the Ohmic spectral density with a frequency cutoff ω_{D}, which defines the dissipation kernel $\gamma(s)$ as

$$J(\omega) = m_0\gamma\omega\frac{\omega^2}{\omega^2+\omega_{\mathrm{D}}^2} \qquad \gamma(s) = \frac{2}{m_0}\int_0^{\infty}\frac{\mathrm{d}\omega}{\pi}\frac{J(\omega)}{\omega}\cos(\omega t),$$

whose Laplace transform $\tilde{\gamma}(|\nu_l|)$ given by

$$\tilde{\gamma}(|\nu_l|) = \frac{\gamma\omega_{\mathrm{D}}}{\omega_{\mathrm{D}}+|\nu_l|}.$$

4. Deviations from Canonical Typicality and Squeezing Generation

From the equilibrium variances given by [Phys. Rep. 168, 115 (1988), Z. Phys. B 55, 87 (1984)], we have the following relation

$$\langle p^2\rangle = m_0^2\omega_0^2\langle q^2\rangle + \Delta,$$

where Δ is responsible for the generation of squeezing and the deviations from canonical typicality.

We discuss the low/high temperature regime in which one can analyze when the canonical Boltzmann distribution can be received at equilibrium.

For Low Temperature: $\hbar\omega_0/k_{\mathrm{B}}T \gg 1$ and $\hbar\gamma/k_{\mathrm{B}}T \gg 1$, we get $\hat{\gamma}(|\nu_l|) \to \gamma$.

Thus, we obtain a non-vanishing damping kernel and as a consequence a deviation from the canonical distribution. Besides, we have that the term responsible for the squeezing generation is given by

$$\Delta \approx \hbar\gamma m_0 \ln(\hbar\omega_{\mathrm{D}}/k_{\mathrm{B}}T),$$

and as a consequence, for low temperatures, the unsqueezed state cannot be recovered.

For High Temperature: $\hbar\omega_0/k_{\mathrm{B}}T \ll 1$ and $\hbar\gamma/k_{\mathrm{B}}T \ll 1$, we get $\hat{\gamma}(|\nu_l|) \to 0$ and $k(\tau) \to 0$.

Therefore, the functional influence is $\mathcal{F}(q) = 1$ and we recover the canonical typicality because $\rho_\beta(q,q')$ is

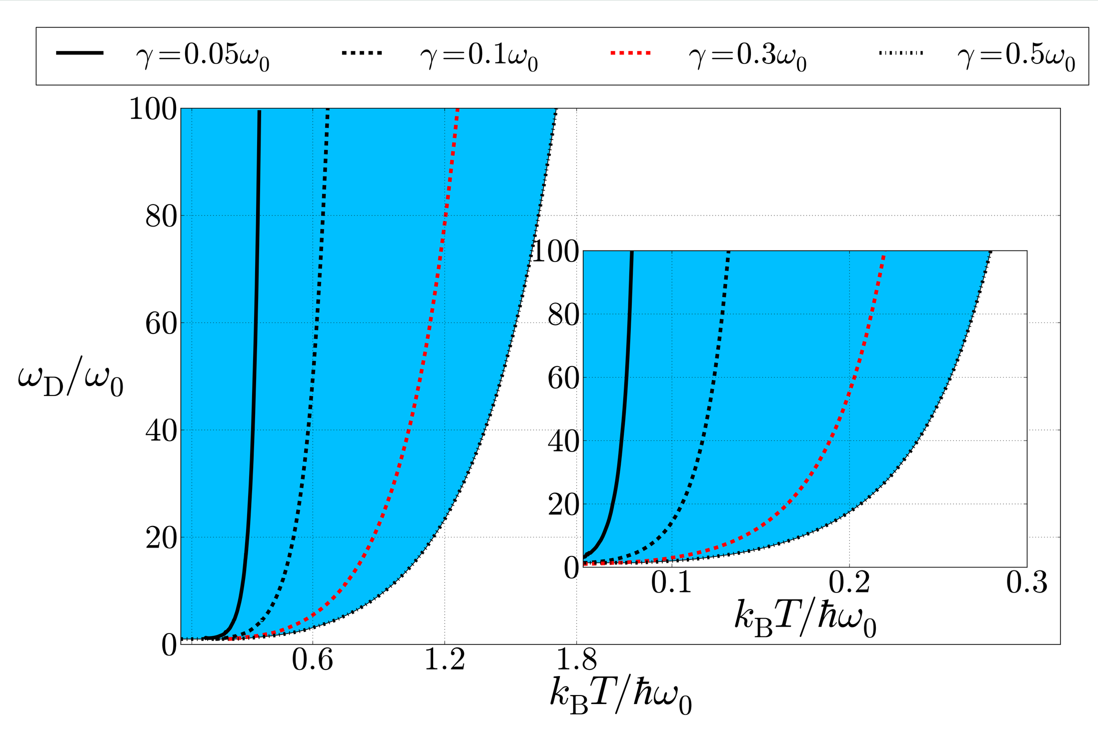
$$\rho_\beta(q,q') = \frac{1}{Z}\int\mathcal{D}q\exp\left(-\frac{1}{\hbar}S_{\mathrm{S}}^{\mathrm{E}}[q]\right).$$

As to the squeezing generation, the term responsible for it, in this limit, adopts the form

$$\Delta \approx \hbar^2\gamma m_0\omega_{\mathrm{D}}/12k_{\mathrm{B}}T.$$

Thus, Δ vanishes at high temperatures and the unsqueezed state is recovered. In nutshell, we do not have deviations from the canonical typicality and squeezing for high temperatures.

5. Partition Function and Entropy



If the coupling between bath and system is higher, we need a lower temperature to get deviations from the canonical partition function Z_{can}, which corresponds to the partition function of the system. Likewise, if the system is non-Markovian (low ω_{D}) we need a lower temperature to get deviations.

We propose that the limit which we get deviations from the canonical quantities is given by

$$\Lambda\omega_0 < 1,$$

where

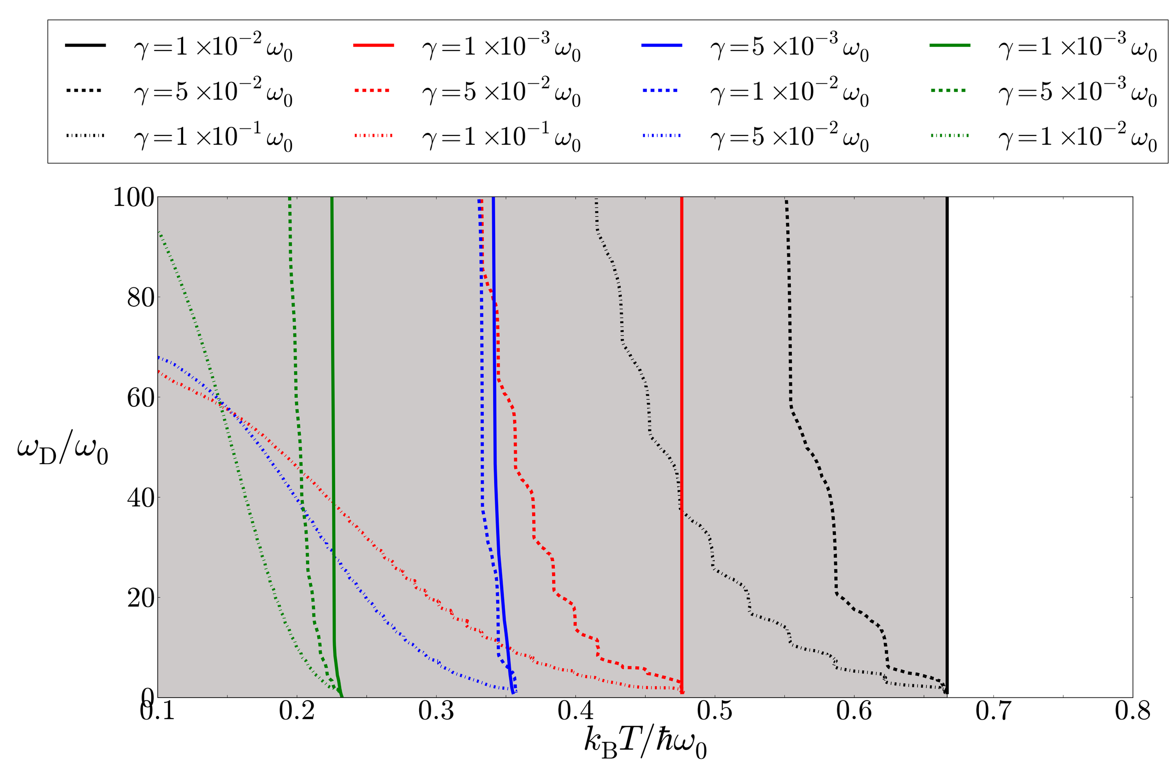
$$\Lambda = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}\frac{1}{\omega_0^2+\nu_{\mathrm{n}}^2+\gamma|\nu_{\mathrm{n}}|\omega_{\mathrm{D}}/\left(\omega_{\mathrm{D}}+|\nu_{\mathrm{n}}|\right)}.$$

6. Entanglement at equilibrium

Consider two identical harmonic oscillators with masses m_0 and frequencies ω_0 linearly coupled with coupling constant c_0. At equilibrium, it is well known that entanglement between these two harmonic oscillators can survive only if $\hbar\omega/k_{\mathrm{B}}T \gg 1$.

For this, we couple each oscillator to its own independent thermal bath in order not to have second order correlations via the bath. The Hamiltonian of the system given by

$$\hat{H} = \frac{\hat{p}_1^2+\hat{p}_2^2}{2m_0} + \frac{1}{2}m_0\omega_0^2(\hat{q}_1^2+\hat{q}_2^2) - c_0\hat{q}_1\hat{q}_2 + \sum_j^{\infty}\sum_{\alpha=1}^{2}\frac{\hat{p}_{j,\alpha}^2}{2m_j} + \frac{m_j\omega_j^2}{2}\left(\hat{q}_{j,\alpha} - \frac{c_j}{m_j\omega_j^2}\hat{q}_\alpha\right)^2,$$



Phase diagram of entanglement in the presence of non-Markovian interaction. We compare the entanglement phase diagram for $c_0 = 0.2\omega_0^2$ (black curves), $c_0 = 0.1\omega_0^2$ (red curves), $c_0 = 0.051\omega_0^2$ (blue curves) and $c_0 = 0.01\omega_0^2$ (green curves). We observe that (i) the stronger the coupling between the oscillators, c_0, the higher the temperature the system can support entanglement at equilibrium; (ii) the higher the damping rate γ, the stronger the influence of the non-Markovian interaction depicted by the ratio $\omega_{\mathrm{D}}/\omega_0$; and (iii) the smaller the ratio $\omega_{\mathrm{D}}/\omega_0$ (a more non-Markovian interaction), the higher the temperature at which the system can support entanglement at equilibrium.

7. Conclusions

Regardless the coupling strength, canonical typicality is achieved at high temperature!
Non-Markovian interactions allows for squeezed thermal states and entangled states at higher temperatures!