Collisional reservoirs and thermalization

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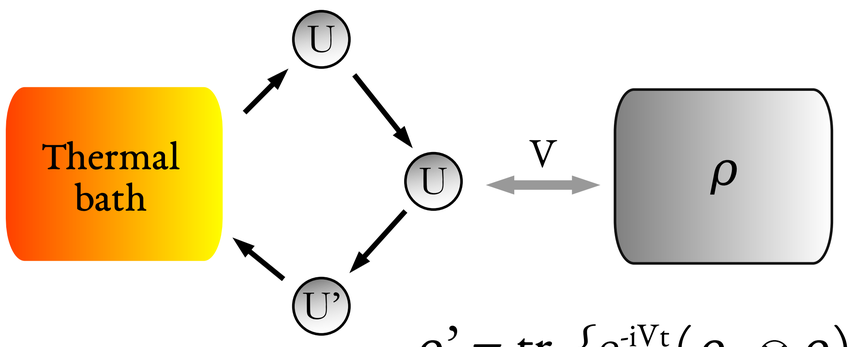
A proper understanding of the interaction between a quantum system and a thermal reservoir is crucial for the development of thermodynamics. Collisional reservoirs are becoming a remarkable tool in this due to their capacity to simulate thermal interactions in a simple way.

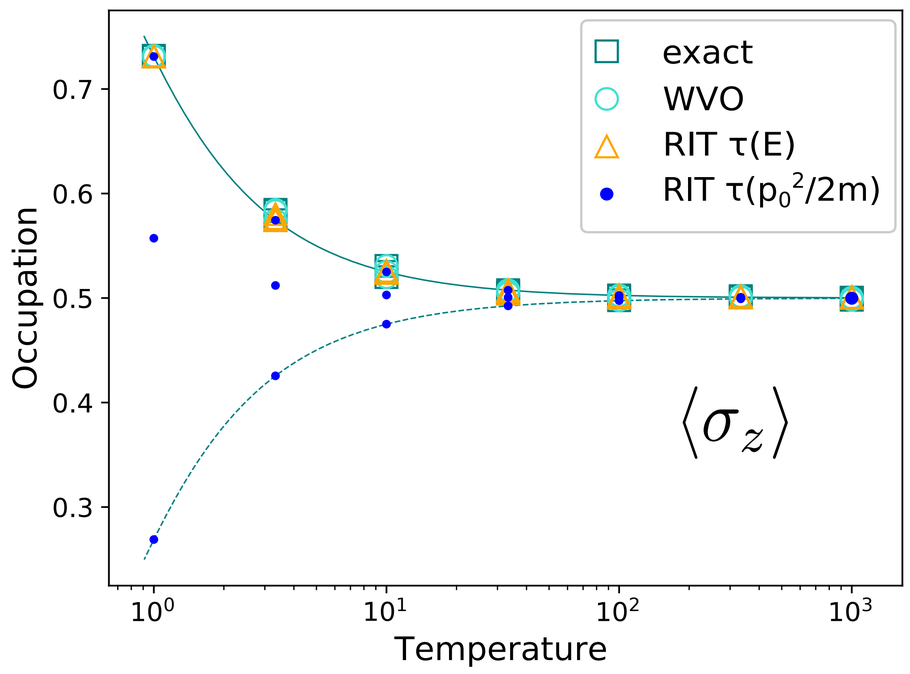
Motivation



$$\rho' = \mathrm{tr}_U\{e^{-iVt}(\rho_U \otimes \rho)\, e^{iVt}\}$$

Common implementation of Collisional reservoirs are based on repeated interactions of the target system (ρ) with ancillary systems (units U) in thermal state. However, the continuous switching on and off of the system-unit interaction could prevent thermalization. [1]

Results [3]



1.- We represent the average occupation of the target in steady state. In the numerical solution of the whole process (exact), the system thermalizes.

2.- For high incident energies, we find the Wave-Vector-Operator approx.

$$t_{J'J}(E) = \begin{cases} e^{-iL(k_J+k_{J'})/2}\langle e_{J'} \mid e^{iL\mathbb{K}(E)} \mid e_J\rangle & \text{if } E > e_{\max} \\ \delta_{J'J} & \text{if } E \le e_{\max} \end{cases} \qquad \mathbb{K}(E) \equiv \sqrt{2m(E-H)}$$

This approximation also thermalizes.

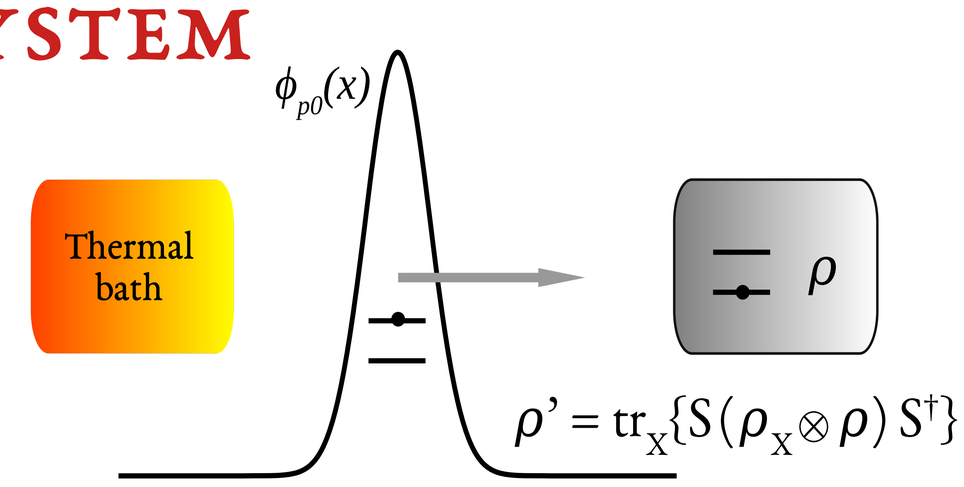
3.- If the kinetic energy scale is larger than that of the internal degrees of freedom, WVO is reduced to a form similar to the usual repeated interaction evolution,

$$t_{J'J}(E) \simeq e^{i\tau(E)[e_{J'}+e_J]/2}\,\langle e_{J'} \mid e^{-i\tau(E)H} \mid e_J\rangle \qquad \tau(E) \equiv \frac{L}{v_E} = \frac{L}{\sqrt{2E/m}}$$

$$v_E \equiv \sqrt{2E/m} = \sqrt{(p_0/m)^2 + 2e_J/m}$$

4.- If we consider $e_J \sim 0$, the system becomes the common repeated interaction thermostat, and thermalization fails

System



We consider both the units and the target as two level systems. Units will also have a kinetic degree of freedom

$$H_{\mathrm{tot}} = \frac{\hat{p}^2}{2m} + \chi_L(\hat{x})H_{US} + H_U + H_S$$

Narrow wave packages ϕ_{p_0} induce a scattering map in system + unit energy levels e_J

$$\rho'_{J'K'} = \sum_{J,K} \mathbb{S}^{JK}_{J'K'}\rho_{JK}$$

$$\mathbb{S}^{JK}_{J'K'} \simeq t_{J'J}(E_{p_0}+e_J)\,[t_{K'K}(E_{p_0}+e_K)]^* + r_{J'J}(E_{p_0}+e_J)\,[r_{K'K}(E_{p_0}+e_K)]^*\ ,$$

where t, r are transition and reflection amplitudes, and E_{p_0} is the kinetic energy.

Conditions for thermalization

Internal states of the units are in thermal equilibrium, and the momentum follows the effusion distribution

$$p_{j_U} = \frac{e^{-\beta e^{(U)}_{j_U}}}{Z_U} \qquad \mu(p) = \frac{\beta|p|}{m}e^{-\beta p^2/(2m)} \qquad p \in [0,\infty]$$

In this case, the states of the system, j_S follow detailed balance [2]

$$p(J \to J') = e^{-\beta\Delta_{J'J}}\int_0^\infty dp'_0\,\frac{\beta p'_0}{m}e^{-\beta p'^2_0/(2m)}P_{JJ'}(p'_0) = e^{-\beta\Delta_{J'J}}p(J' \to J)$$

$$p(j_S \to j'_S) = e^{-\beta\left[e^{(S)}_{j'_S} - e^{(S)}_{j_S}\right]}p(j'_S \to j_S)$$

Conclusions

1.- We present a model of a genuine quantum collisional thermostat:

→ The external degree of freedom provides the required energy for the switching on and off of the interaction. If the units come from a thermal reservoir, then, the energy exchange is no more work, but heat, and the target thermalizes.

→ It can be treated both numerically and analitically in a relatively simple way.

2.- The model can be easily related with common implementations of collisional thermostats, helping us to understand the causes of the failure of thermalization.

[1] Barra, F. (2015). The thermodynamic cost of driving quantum systems by their boundaries. Scientific reports, 5(1), 1-10.

[2] Ehrich, J., Esposito, M., Barra, F., Parrondo, J. M. (2020). Micro-reversibility and thermalization with collisional baths. Physica A: Statistical Mechanics and its Applications, 552, 122108.

[3] Tabanera, J., Luque, I., Jacob, S. L., Esposito, M., Barra, F., Parrondo, J. M. (2022). Quantum collisional thermostats. New Journal of Physics.

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