Generalized Effective Quantum Thermodynamics

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Introduction

- We consider the time-dependent observables in resonance with ”free” Hamiltonian.
- We consider the long time scale with respect to this ”free” Hamiltonian, such that fast oscillations could be neglected and only slow observables could be actually observed.
- Under such conditions the usual Gibbs state is equivalent to the one obtained by averaging with respect to ”free” dynamics.

More details could be found in **arXiv:2110.14407**.

Time-dependent observables and long timescale

- We consider the Hamiltonian of the form

$$H = H_0 + \lambda H_I$$

- An observable depends on time in such a way that it is constant in the interaction picture

$$A(t) = e^{-iH_0 t} A e^{iH_0 t}$$

  i.e. it equals A in the interaction picture for ”free” Hamiltonian H_0. So $A(t)$ is in resonance with H_0. This is a usual situation in the case of spectroscopy, for example.
- We are interested in long timescale such that

$$\omega t \gg 1$$

  for all non-zero Bohr frequencies ω of H_0.
- A is assumed to be time-independent just for simplicity. It is also possible to assume that A is slow (with respect to non-zero Bohr frequencies) varying in time.

Effective Gibbs state and effective Hamiltonian

Canonical Gibbs state

$$\rho_\beta = \frac{e^{-\beta H}}{Z}$$

For long timescale we obtain

$$\operatorname{Tr} A(t) \rho_\beta \approx \operatorname{Tr} A \mathcal{P} \rho_\beta,$$

where

$$\mathcal{P}\rho = \lim_{T \to +\infty} \frac{1}{T} \int_0^T e^{iH_0 t} \rho e^{-iH_0 t} dt$$

Effective Gibbs state for slow observables

$$\tilde{\rho}_\beta = \mathcal{P}\rho_\beta = \frac{1}{Z} e^{-\beta \tilde{H}},$$

where $\tilde{H}$ is an effective (thermal) Hamiltonian for slow observables.

Let us remark that $Z \equiv e^{-\beta H} = \operatorname{Tr} e^{-\beta \tilde{H}}$.

Equilibrium effective thermodynamics

Similarly to usual formulae for entropy and internal energy

$$S = -\operatorname{Tr} \rho_\beta \ln \rho_\beta, \qquad U = \operatorname{Tr} H \rho_\beta,$$

let us define their effective analogs

$$\tilde{S} = -\operatorname{Tr} \tilde{\rho}_\beta \ln \tilde{\rho}_\beta, \qquad \tilde{U} = \operatorname{Tr} \tilde{H} \tilde{\rho}_\beta.$$

They are related by the following formulae

$$S = \tilde{S} - \Delta S, \qquad U = \tilde{U} - \Delta U,$$

where the corrections have exactly the same form as in the mean force Hamiltonian theory:

$$\Delta S = -\beta^2 \langle \partial_\beta \tilde{H} \rangle_\sim, \qquad \Delta U = -\beta \langle \partial_\beta \tilde{H} \rangle_\sim = \beta^{-1} \Delta S.$$

Here $\langle \cdot \rangle_\sim$ denotes the average with respect to the effective Gibbs state, i.e. $\langle \cdot \rangle_\sim \equiv \operatorname{Tr}(\cdot \, \tilde{\rho}_\beta)$.
In particular, the equilibrium free energy is the same both for exact and effective Gibbs states

$$F \equiv U - \beta^{-1} S = \tilde{U} - \beta^{-1} \tilde{S} \equiv \tilde{F}.$$

It is possible to prove that

$$\Delta S \geq 0, \qquad \Delta U = \beta^{-1} \Delta S \geq 0.$$

$\tilde{S}$ and $\tilde{U}$ could be interpreted as entropy and as energy which are accessible to our observations. Our observable entropy is $\tilde{S}$, but due to our restricted observational capabilities we have the information loss quantified by ΔS. This information loss comes with energy loss quantified by ΔU and is hidden from our observations. But the equilibrium free energy is invariant under our observational capabilities.

Non-equilibrium effective thermodynamics

Similarly to exact non-equilibrium free energy

$$F_\rho = \langle H \rangle + \beta^{-1} \langle \ln \rho \rangle,$$

where $\langle \cdot \rangle \equiv \operatorname{Tr}(\rho \, \cdot)$, one can define

$$\tilde{F}_\rho \equiv \langle \tilde{H} \rangle_{\mathcal{P}} + \beta^{-1} \langle \ln \mathcal{P}\rho \rangle_{\mathcal{P}} = F + \beta^{-1} S(\mathcal{P}\rho || \tilde{\rho}_\beta),$$

where $\langle \cdot \rangle_{\mathcal{P}} \equiv \operatorname{Tr}(\mathcal{P}\rho \, \cdot)$.
Then it is possible to write

$$F_\rho = \tilde{F}_\rho + \Delta F_\rho,$$

where ΔF_ρ has a definite sign, namely

$$\Delta F_\rho = \beta^{-1}(S(\rho||\rho_\beta) - S(\mathcal{P}\rho||\mathcal{P}\rho_\beta)) \geq 0,$$

where $S(\rho||\sigma)$ is relative entropy. Thus, in the non-equilibrium case the free energy is non-invariant under observational capabilities and we have additional free energy cost ΔF_ρ.

Analogy with the mean force Hamiltonian

The mean force Hamiltonian is closely related to the projector

$$\mathcal{P}' = \operatorname{Tr}_B(\cdot) \otimes \rho_B$$

Then

$$\mathcal{P}' \frac{e^{-\beta H}}{Z} = \frac{1}{Z} \operatorname{Tr}_B e^{-\beta H} \otimes \frac{1}{Z_B} e^{-\beta H_B} = \frac{1}{Z_{\text{mf}}} e^{-\beta H_{\text{mf}}} \otimes \frac{1}{Z_B} e^{-\beta H_B},$$

where $Z_{\text{mf}} = Z / Z_B$. Thus, a stricter analog of our effective Hamiltonian should be $H_{\text{mf}} + H_B$ with partition function Z. But it seems that for operational meaning of the mean force Hamiltonian the information about H_B is also important, which makes this analog more natural.
This suggests that such an effective thermodynamics ***could be generalized to arbitrary projectors***, which includes both this work with the projector $\mathcal{P}$ and mean force Hamiltonian theory with the projector $\mathcal{P}'$ as particular cases.

Perturbative formulae

For explicit calculations it is useful to expand the interaction Hamiltonian in the following way

$$H_I = \sum_\omega D_\omega, \qquad [H_0, D_\omega] = -\omega D_\omega,$$

Then the effective Hamiltonian takes the form

$$\tilde{H} = \underbrace{H_0 + \lambda D_0}_{RWA} \underbrace{- \lambda^2 \sum_{\omega \neq 0} \frac{\beta\omega + e^{-\beta\omega} - 1}{\beta \omega^2} D_\omega D_\omega^\dagger}_{temperature-dependent\ correction} + O(\lambda^3),$$

which leads to the following expansions

$$\Delta S = \sum_{\omega > 0} \frac{1 - e^{-\beta\omega}}{\beta\omega} \langle D_\omega D_\omega^\dagger \rangle_0 + O(\lambda^3),$$

$$\Delta U = \sum_{\omega > 0} \frac{1 - e^{-\beta\omega}}{\beta^2 \omega} \langle D_\omega D_\omega^\dagger \rangle_0 + O(\lambda^3),$$

where $\langle \cdot \rangle_0$ is the average with respect to Gibbs state at $\lambda = 0$, and

$$\Delta F_{\tilde{\rho}_\beta} = \langle H_{\text{RWA}} - \tilde{H} \rangle_\sim = \Delta U + O(\lambda^3).$$

Simple example

Let us consider the two interacting two-level systems a and b

$$H = \omega_a \sigma_a^+ \sigma_a^- + \omega_b \sigma_b^+ \sigma_b^- + \lambda(\sigma_a^- + \sigma_a^+)(g^* \sigma_b^- + g \sigma_b^+),$$

where $\omega_a > 0$, $\omega_b > 0$ and $\sigma_i^\pm$ are usual ladder operators for two-level systems $i = a, b$.
1) Off-resonance case $\omega_a \neq \omega_b$.

$$\Delta S_{\text{off-res}} = \lambda^2 \beta |g|^2 \frac{\omega_a \tanh \frac{\beta\omega_a}{2} - \omega_b \tanh \frac{\beta\omega_b}{2}}{\omega_a^2 - \omega_b^2} + O(\lambda^3).$$

2) Resonance case $\omega_b = \omega_a + \lambda \delta\omega$.

$$\Delta S_{\text{res}} = \lambda^2 \beta |g|^2 \frac{\tanh \frac{\omega_a \beta}{2}}{2\omega_a} + O(\lambda^3)$$

Let us remark that it does not coincide with the off-resonance case with $\omega_b \to \omega_a$. Namely, we have

$$\Delta S_{\text{off-res}}|_{\omega_b \to \omega_a} = \Delta S_{\text{res}} + \lambda^2 \left(\frac{\beta |g|}{2 \cosh \frac{\beta\omega_a}{2}} \right)^2 + O(\lambda^3).$$

Thus, off-resonance averaging leads to larger information loss in the ”resonance” limit than resonance averaging.

Conclusions

1. We have introduced effective Gibbs state and effective Hamiltonian for averaged observables and have defined both equilibrium and non-equilibrium effective thermodynamic quantities.
2. We have shown that differences between effective and exact thermodynamic quantities have definite sign.
3. We have shown that our approach could be generalized for other projectors.
4. We have presented perturbative formulae both for the effective Hamiltonian and the effective thermodynamic quantities.