Perturbation theory for effective Gibbs state

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Outline

Time-dependent observables and long timescale

- We consider the Hamiltonian of the form

$$H = H_0 + \lambda H_I$$

- Observable depends on time in such a way that it are 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.

Time-dependent observables and long timescale

- 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 observe only the long-time averages

$$\lim_{T \to +\infty} \frac{1}{T} \int_0^T \langle A(t) \rangle = \operatorname{Tr} A \mathcal{P} \rho_\beta,$$

where

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

$H_0 = \sum_\varepsilon \varepsilon \Pi_\varepsilon$.

Effective Gibbs state and effective Hamiltonian

Effective Gibbs state for slow observables

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

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

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

Main result

Theorem 1

The following asymptotic expansion holds

$$\tilde{H} = H_0 + \sum_{n=1}^{\infty} \lambda^n \kappa_n,$$

$$\kappa_n \equiv -\beta^{-1} \sum_{k_0+\dots+k_m=n, k_0 \geqslant 1} \frac{(-1)^m}{m+1} \mathcal{M}_{k_0}(\beta)\mathcal{M}_{k_1}(\beta) \cdots \mathcal{M}_{k_m}(\beta),$$

$$\mathcal{M}_k(\beta) \equiv (-1)^k \int_0^{\beta} d\beta_1 \dots \int_0^{\beta_{k-1}} d\beta_k \mathcal{P} H_I(\beta_1) \dots H_I(\beta_k),$$

$$H_I(\beta) \equiv e^{\beta H_0} H_I e^{-\beta H_0},$$

if $\mathcal{M}_k(\beta)$ are well-defined.

Eigenoperator expansion

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

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

which leads to

$$\mathcal{P} H_I(\beta_1) \cdots H_I(\beta_k) = \sum_{\omega_1,\ldots,\omega_{k-1}} e^{-(\beta_1-\beta_k)\omega_1-\ldots-(\beta_{k-1}-\beta_k)\omega_{k-1}} D_{\omega_1} \cdots D_{\omega_{k-1}} D_{-\omega_1-\ldots-\omega_{k-1}}$$

Eigenoperator expansion

In particular, the first terms of the cumulant expansion take the form

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

Simple example

$$H = Ea^\dagger a + \omega_1 b^\dagger b + \lambda(a + a^\dagger)(g^* b + g b^\dagger)$$

- $E \neq \omega_1$ (off-resonance)

$$\begin{aligned}\tilde{H} =& E n_a + \omega_1 n_b + \lambda^2 \beta |g|^2 \biggl(\frac{1}{2}(2n_a + 1)(2n_b + 1) \\ & + f(\beta(\omega_1 - E))(n_a + 1)n_b + f(\beta(E - \omega_1))n_a(n_b + 1) \\ & + f(-\beta(E + \omega_1))(n_a + 1)(n_b + 1) + f(\beta(E + \omega_1))n_a n_b \biggr)\end{aligned}$$

where $f(x) \equiv \frac{e^x - \left(1 + x + \frac{x^2}{2}\right)}{x^2}$, $n_a = a^\dagger a$, $n_b = b^\dagger b$.

Simple example

In particular, in high-temperature limit

$$\tilde{H} = Ea^\dagger a + \omega_1 b^\dagger b + \lambda^2 |g|^2 \frac{\beta}{2}(2n_a + 1)(2n_b + 1)$$

Simple example

- $E = \omega_1$ (resonance)

$$\begin{aligned}\tilde{H} = &E(a^\dagger a + b^\dagger b) + \lambda(g^* a^\dagger b + g a b^\dagger)\\ &+ \lambda^2 \beta |g|^2 \Bigg(\frac{1}{2}((n_a + 1)(n_b + 1) + n_a n_b) + \\ &+ f(-\beta(E + \omega_1))(n_a + 1)(n_b + 1) + f(\beta(E + \omega_1)) n_a n_b \Bigg)\end{aligned}$$

Simple example

- $E = \omega_1 + O(\lambda)$ (non-strict resonance)

$$
\begin{aligned}
\tilde{H} =& E a^\dagger a + \omega_1 b^\dagger b + \lambda (g^* a^\dagger b + g a b^\dagger) \\
& + \lambda^2 \beta |g|^2 \left(\frac{1}{2}((n_a + 1)(n_b + 1) + n_a n_b) + \right. \\
& \left. + f(-\beta(E + \omega_1))(n_a + 1)(n_b + 1) + f(\beta(E + \omega_1)) n_a n_b \right)
\end{aligned}
$$

Mean force Hamiltonian for effective Gibbs state

$$\mathrm{Tr}_B\,\mathcal{P}\rho_\beta = \frac{1}{\tilde{Z}_{mf}} e^{-\beta \tilde{H}_{mf}}, \qquad \tilde{Z}_{mf} = \mathrm{Tr}_S\, e^{-\beta \tilde{H}_{mf}}$$

$$\tilde{H}_{mf} = H_S + \sum_{n=1} \lambda^n k_n,$$

$$k_n = -\beta^{-1} \sum_{k_0+\dots+k_m=n, k_0 \geqslant 1} \frac{(-1)^m}{m+1} \langle \mathcal{M}_{k_0}(\beta) \rangle_B \langle \mathcal{M}_{k_1}(\beta) \rangle_B \cdots \langle \mathcal{M}_{k_m}(\beta) \rangle_B$$

where $\langle \,\cdot\, \rangle_B \equiv \mathrm{Tr}_B(\,\cdot\, Z_B^{-1} e^{-\beta H_B})$, $Z_B = \mathrm{Tr}_B\, e^{-\beta H_B}$.

Mean force Hamiltonian for effective Gibbs state

Let

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

then

$$\tilde{H}_{mf} = H_S + \lambda \langle D_0 \rangle_B + \lambda^2 \Bigg(\sum_{\omega \neq 0} \frac{\beta\omega + e^{-\beta\omega} - 1}{\beta\omega^2} \langle D_{\omega} D_{-\omega} \rangle_B + \frac{\beta}{2} (\langle D_0^2 \rangle_B - \langle D_0 \rangle_B^2) \Bigg) + O(\lambda^3)$$

Mean force Hamiltonian for effective Gibbs state

Let

$$D_\omega = \sum_{\omega_1} S_{\omega-\omega_1} \otimes B_{\omega_1}, \qquad [H_S, S_\omega] = -\omega S_\omega, \qquad [H_B, B_\omega] = -\omega B_\omega$$

then

$$\tilde{H}_{mf} = H_S + \lambda \sum_{\omega} \langle B_{-\omega} \rangle_B S_\omega +$$

$$+\lambda^2 \sum_{\omega_1,\omega_2} \Bigg(\sum_{\omega \neq 0} \frac{\beta\omega + e^{-\beta\omega} - 1}{\beta\omega^2} \langle B_{\omega-\omega_1} B_{-\omega-\omega_2} \rangle_B$$

$$+\frac{\beta}{2} (\langle B_{-\omega_1} B_{-\omega_2} \rangle_B - \langle B_{-\omega_1} \rangle_B \langle B_{-\omega_2} \rangle_B) \Bigg) S_{\omega_1} S_{\omega_2} + O(\lambda^3)$$

Mean force Hamiltonian for effective Gibbs state

In particular, if $H_I = (S + S^\dagger) \otimes \sum_\omega (B_\omega + B_\omega^\dagger)$, $S \equiv S_E$, $\langle B_\omega \rangle_B = 0$, $\langle B_{\omega_1} B_{\omega_2} \rangle_B = 0$, then

$$\tilde{H}_{mf} = H_S + \lambda^2 (g_\beta(E) S^\dagger S + g_\beta(-E) S S^\dagger) + O(\lambda^3)$$

$$g_\beta(E) = \sum_\omega \frac{\beta\omega + e^{-\beta\omega} - 1}{\beta\omega^2} \langle B_{\omega - E} B_{\omega - E}^\dagger \rangle_B$$

Conclusion

- $\tilde{H} = H_0 + \sum_{n=1}^{\infty} \lambda^n \kappa_n$
- $\tilde{H}_{mf} = H_S + \sum_{n=1} \lambda^n k_n$

Thank you for your attention!