Ohmic vs Markovian heat bath — two-page-tutorial

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In open quantum system theory the Ohmic heat bath and the Markovian heat bath are two different but closely related special cases. We discuss them on a common bases.

I. HEAT BATH: COORDINATE COUPLING

System-Bath total Hamiltonian: $\hat{H}_S + \hat{H}_B + \hat{H}_I$.

$$\begin{aligned} \hat{H}_S &= \frac{\hat{p}^2}{2M} + V(\hat{q}), \\ \hat{H}_B &= \sum \left(\frac{\hat{p}_\alpha^2}{2m_\alpha} + \frac{1}{2} m_\alpha \omega_\alpha^2 \hat{x}_\alpha^2 \right) = \sum \hbar\omega_\alpha \hat{b}_\alpha^\dagger \hat{b}_\alpha, \\ \hat{H}_I &= -\hat{q} \sum c_\alpha \hat{x}_\alpha = -\hat{q} \sum g_\alpha (\hat{b}_\alpha + \hat{b}_\alpha^\dagger) = -\hat{q}\hat{X}, \end{aligned}$$

where $\hat{X} = \sum c_\alpha \hat{x}_\alpha = \sum g_\alpha (\hat{b}_\alpha + \hat{b}_\alpha^\dagger)$ is called the B-field. The two conventions of coupling constants are related by $c_\alpha = \sqrt{2m_\alpha\omega_\alpha/\hbar}\, g_\alpha$.

Theorem: If at $t = 0$ the initial states of S and B are uncorrelated and B is in thermal equilibrium (at a certain inverse temperature $\beta = 1/k_B T$) then the reduced dynamics of S for $t > 0$ is completely determined by $\hat{H}_S$ and the equilibrium correlation

$$C_{XX}(t-u) = \langle \hat{X}_t \hat{X}_u \rangle_\beta$$

where $\hat{X}_t$ is the B-field in interaction picture.

This correlation is uniquely determined by the effective spectral density

$$J(\omega) = \frac{\pi}{\hbar} \sum g_\alpha^2 \delta(\omega - \omega_\alpha)$$

which encodes the coupling constants as well. [With the spectral density itself, $n(\omega) = \frac{\pi}{\hbar}\sum \delta(\omega - \omega_\alpha)$, the effective spectral density takes the form $J(\omega) = ((g(\omega))^2 n(\omega)$ where $g(\omega)$ is the frequency-smoothened form of g_α.] We can express $C_{XX}(t)$ via $J(\omega)$:

$$C_{XX}(t) = \frac{\hbar}{\pi} \int_0^\infty J(\omega) \left(\coth(\frac{\hbar\beta\omega}{2}) \cos(\omega t) - i \sin(\omega t) \right) d\omega.$$

The imaginary part is purely dynamical, independent of T.

To describe the reduced dynamics of S, either the general (non-Markovian) master equation for the reduced density matrix $\hat{\rho}$ or the Heisenberg equation of $\hat{q}$ can be used. With the second option, the following non-Markovian quantum Langevin equation can be derived ('Lamb-shift' in $\hat{H}_S$ and the 'initial slip' are ignored):

$$M\ddot{\hat{q}}(t) = -V'(\hat{q}) - M \int_0^t \gamma(t-t') \dot{\hat{q}}(t') dt' + \hat{X}_t$$

where the damping term is determined by the memory kernel $\gamma(t - t')$ which is independent of $\hbar$ and of T:

$$M\gamma(t) = \frac{2}{\pi} \int_0^\infty \frac{J(\omega)}{\omega} \cos(\omega t) d\omega.$$

II. OHMIC DAMPING

The Ohmic model applies when damping force is proportional to the instant velocity. Ohm's Law in electricity results from such microscopic damping force on electrons moving in a potential. If we are interested in such memory-less damping, we must assume the Ohmic effective spectral density $J(\omega) = \eta\omega$ (with high-frequency cutoff ω_c) when the memory disappears from the damping kernel: $M\gamma(t) = 2\eta\delta(t)$. The quantum Langevin equation of motion becomes

$$M\ddot{\hat{q}} = -V'(\hat{q}) - \eta\dot{\hat{q}} + \hat{X}_t,$$

η is the damping (friction) constant. The fluctuation force $\hat{X}_t$ is a *colored quantum* noise of correlation $C_{XX}(t - t')$ hence the corresponding reduced dynamics remains non-Markovian!

However, at higher T the real part of the Ohmic correlation dominates, the imaginary part can be ignored. We can replace the operator force $\hat{X}_t$ by the *classical* colored noise force X_t:

$$M\ddot{\hat{q}} = -V'(\hat{q}) - \eta\dot{\hat{q}} + X_t.$$

In the high-T limit $\beta \to 0$, the correlation tends to be time-local: $\beta C_{XX}(t) \to 2\eta\delta(t)$. Thus the random force X_t becomes a classical *white*-noise:

$$\langle X_t X_u \rangle_{stoch} = 2\eta k_B T \delta(t-u).$$

Now, replacing $\hat{q}$ by q would yield the classical Langevin equation, its solution $q(t)$ at $V = 0$ would be the Ornstein-Uhlenbeck stochastic process which is non-Markovian itself. Fortunately, the pair of phase space coordinates satisfy Markovian equations (let's go back to the quantum case):

$$\begin{aligned} \dot{\hat{q}} &= \hat{p}/M \\ \dot{\hat{p}} &= -V'(\hat{q}) - \eta\hat{p}/M + X. \end{aligned}$$

Hence the Ohmic (or high-T) dynamics is often called Markovian. The classical Langevin equations do not preserve the canonical commutation relations between q and p, yet nobody cares because this follows duely from the irreversible modification of the canonical dynamics. In the quantum case, however, the issue $[\hat{q}, \hat{p}] \neq i\hbar$ is a fatal error, the above quantum Langevin equation with the classical white-noise X_t can be totally incorrect e.g. for certain minimum uncertainty wave packets.

III. HEAT BATH: GENERAL COUPLING

$\hat{H}_S$ is arbitrary, $\hat{H}_B$ is the same as before,

$$\hat{H}_I = \hat{s}^\dagger \sum g_\alpha \hat{b}_\alpha + s \sum g_\alpha \hat{b}_\alpha^\dagger = \hat{s}^\dagger B + h.c.$$

where $\hat{B}$ is the non-Hermitian bosonic B-field:

$$\hat{B} = \sum g_\alpha \hat{b}_\alpha.$$

E.g.: $\hat{s} = -\hat{q} - i\chi\hat{p}$ yields $\hat{H}_I = -\hat{q}\hat{X} - \chi\hat{p}\hat{Y}$ where $\hat{X} = \hat{B} + \hat{B}^\dagger, \hat{Y} = -i(\hat{B} - \hat{B}^\dagger)$, i.e., the coordinate *and* the momentum of S couple to the coordinates *and* momenta of B. [We could have considered complex couplings $g_\alpha \neq g_\alpha^*$ but it turns out that the reduced dynamics of S wouldn't depend on the phases of g_α.]

The same *Theorem* holds as before. Starting from uncorrelated S and B, the equilibrium correlations of the B-fields $\hat{B}, \hat{B}^\dagger$ (or $\hat{X}, \hat{Y}$), together with $\hat{H}_S$ and β, will fully determine the reduced dynamics of S.

All non-vanishing correlations are determined by the effective spectral density and the temperature.

$$C_{B^\dagger B}(t) = \langle \hat{B}_t^\dagger \hat{B} \rangle_\beta = \frac{\hbar}{\pi} \int J(\omega) \frac{\exp(i\omega t)}{\exp(\hbar\beta\omega)-1} d\omega$$

$$C_{BB^\dagger}(t) = \langle \hat{B}_t \hat{B}^\dagger \rangle_\beta = \frac{\hbar}{\pi} \int J(\omega) \frac{\exp(-i\omega t)}{1-\exp(-\hbar\beta\omega)} d\omega$$

IV. MARKOVIAN CASE

At $T > 0$ the correlations cannot become time-local in general. If, however, the range of the relevant (coupled) part of the spectrum of $\hat{H}_S$ is finite then we can introduce Markovian effective spectral densities.

First, we assume zero temperature ($\beta = \infty$) where $C_{B^\dagger B}$ vanishes while $C_{BB^\dagger}$ becomes time-local,

$$C_{BB^\dagger}(t) = 2\hbar J \delta(t)$$

provided we extend the spectrum of B for negative frequencies as well and choose flat effective spectral density $J(\omega) = J$. This is correct if the true effective spectral density is unstructured (flat) over the finite range of the relevant frequencies. The chosen abstract B with $J(\omega) = J$ may be called Markovian. The reduced dynamics of S becomes Markovian. If this time, instead of the Langevin equation, we use the alternative math to describe the reduced dynamics of S, we can derive the following master equation:

$$\dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H}_S, \hat{\rho}] - \frac{J}{\hbar}\left(2\hat{s}\hat{\rho}\hat{s}^\dagger - \{\hat{s}^\dagger\hat{s}, \hat{\rho}\}\right).$$

That's the standard Markovian master equation in the Lindblad form.

Second, we consider Markovianity at finite T as well. We assume discrete spectrum of $\hat{H}_S$ and, for simplicity, we couple a single transition to B:

$$\hat{s} = |1\rangle\langle 2|, \quad \omega_2 - \omega_1 = \epsilon/\hbar > 0.$$

We retain the flat Markovian effective spectrum $J(\omega) = J$ as before and, as a further approximation, we ignore the frequency dependence of the thermal factors in the relevant vicinity of $\omega = \epsilon/\hbar$. Then both correlation functions become time-local:

$$C_{B^\dagger B}(t) = e^{-\beta\epsilon} C_{BB^\dagger}(t) = \frac{2\hbar J}{\exp(\beta\epsilon) - 1}\delta(t).$$

They contribute to the following master equation:

$$\dot{\hat{\rho}} = -\tfrac{i}{\hbar}[\hat{H}_S, \hat{\rho}] + \Gamma\left(\hat{s}\hat{\rho}\hat{s}^\dagger - \tfrac{1}{2}\{\hat{s}^\dagger\hat{s}, \hat{\rho}\}\right) + \\ + e^{-\beta\epsilon}\Gamma\left(\hat{s}^\dagger\hat{\rho}\hat{s} - \tfrac{1}{2}\{\hat{s}\hat{s}^\dagger, \hat{\rho}\}\right).$$

$\Gamma = \hbar^{-1} J/(1 - e^{-\beta\epsilon})$ is the decay constant. If more than a single transition is coupled to B, the extension of the model is possible just by adding similar terms to $\hat{H}_I$, yielding similar Lindblad terms in the above Markovian master equation.

V. OHMIC VS MARKOVIAN

We saw the special case of coordinate coupling $\hat{s} = -\hat{q}$ in Ohmic effective spectrum

$$J(\omega) = \eta\omega, \quad 0 < \omega < \omega_c$$

which case becomes Markovian asymptotically for $\hbar\beta \to 0$, i.e., in the high-T limit. When we retain couplings of both B-coordinates and B-momenta to S, we can achieve quantum Markovianity at any T at a radically different choice

$$J(\omega) = J, \quad -\infty < \omega < \infty$$

called Markovian effective spectrum. The two mathematical models of Markovianity apply in two different physical situations respectively, whose relationship is yet to be clarified.

[1] U. Weiss: Quantum Dissipative Systems (World Scientific, Singapore, 1999).

[2] C. W. Gardiner and P. Zoller: Quantum Noise (Springer, Berlin, 2004).