Hamiltonian of Mean Force From Influence Functional

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SETUP

We're going to at least approximately derive an expression for the Hamiltonian of mean force, using the influence functional formalism in imaginary time. Our starting point is the Caldeira-Leggett model (where we anticipate the path integral by writing it in coordinate form):

$$H_{\rm tot}(q,x) = H_Q(q) + \frac{1}{2}\sum_{\lambda=1}^{M}\left(\dot{x}_\lambda^2 + \omega_\lambda^2 x_\lambda^2\right) - f(q)\sum_\lambda x_\lambda \tag{1}$$

describing a system Q coupled to a bath of oscillators with a bilinear coupling, where $f(q)$ is an arbitrary function of the system coordinates.

In order to obtain the Hamiltonian of mean force, we're going to apply the influence functional formalism to the joint thermal state, which will be represented as a path integral in imaginary time. First, note that the thermal density matrix may be expressed as a propagator in *imaginary time*:

$$\hat{U}(-i\hbar\beta) = \mathrm{e}^{-\beta\hat{H}} = Z_\beta\hat{\rho}_\beta \tag{2}$$

where $\hat{\rho}_\beta$ is the thermal density matrix and Z_β is its partition function. Here, β is a parameter that we can split into arbitrarily many pieces Δ, with $\Delta = \hbar\beta/N$. Now the density matrix is expressible as

$$\rho_\beta = \frac{1}{Z_\beta}\left(\mathrm{e}^{-\frac{\Delta}{\hbar}H}\right)^N. \tag{3}$$

Performing a Trotter splitting as before yields:

$$\rho_\beta(x,x') = \frac{1}{Z_\beta}\lim_{N\to\infty}\int \mathrm{d}x_1 ... \mathrm{d}x_{N-1}\left(\frac{m}{2\pi i\hbar\Delta}\right)^{N/2}\exp\left[-\frac{\Delta}{\hbar}\sum_{j=0}^{N-1}\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\Delta}\right)^2 + V(x_j)\right]\right] \tag{4}$$

using $x = x_0$, $x' = x_N$. The shorthand for this integral is

$$\rho(x,x') = \frac{1}{Z_\beta}\int \mathcal{D}\bar{x}(\tau)\,\mathrm{e}^{-\frac{1}{\hbar}S^E} \tag{5}$$

where S^E is the *Euclidean action*

$$S^E = \int_0^{\hbar\beta}\mathrm{d}\tau\ \left(\frac{1}{2}m\dot{\bar{x}}^2(\tau) + V(\bar{x}(\tau))\right). \tag{6}$$

Applying this to the Caldeira-Leggett Hamiltonian, and performing the usual tricks to integrate out the environment, we obtain the imaginary time path integral describing the reduced equilibrium density matrix in terms of a stochastic average over realisations r. Using $\bar{q}$ to denote a coordinate in imaginary time, we have:

$$\langle \bar{q} \,|\hat{\rho}_\beta|\, \bar{q}' \rangle = \langle \tilde{\rho}(\bar{q};\bar{q}') \rangle_r \tag{7}$$

$$\tilde{\rho}_0(\bar{q};\bar{q}') = \frac{1}{Z_\beta} \int_{\bar{q}(0)=\bar{q}'}^{\bar{q}(\hbar\beta)=\bar{q}} \mathcal{D}\bar{q}\,(\tau) \exp\left[-\frac{1}{\hbar}\tilde{S}^E\left[\bar{q}\,(\tau)\right]\right] \equiv \langle \bar{q}\,|\tilde{\rho}_0|\,\bar{q}' \rangle \,. \tag{8}$$

where

$$\tilde{S}^E\left[\bar{q}\,(\tau)\right] = \int_0^{\hbar\beta} \mathrm{d}\tau \,\; \left(H_Q\left[\bar{q}\,(\tau)\right] + \bar{\mu}\,(\tau)\,\bar{f}\left[\bar{q}\,(\tau)\right]\right). \tag{9}$$

Note that $\bar{\mu}\,(\tau)$ is a noise defined by the correlation

$$\langle \bar{\mu}\,(\tau)\,\bar{\mu}\,(\tau') \rangle_r = \hbar \int_0^\infty \frac{\mathrm{d}\omega}{\pi}\, I\,(\omega)\, \frac{\cosh\left(\omega\left(\frac{\hbar\beta}{2} - \tau + \tau'\right)\right)}{\sinh\left(\frac{1}{2}\beta\hbar\omega\right)} \equiv K_{\bar{\mu}\bar{\mu}}\,(\tau - \tau') \tag{10}$$

Further details of how this is derived can be found in Refs [1, 2].

From this setup, we'd like to go backwards, finding the propagator which corresponds to this imaginary time path integral, and hence the Hamiltonian of mean force. This is slightly complicated by the fact that our noise is *explicitly* imaginary time dependent, so while it's easy to guess the operational form of the propagator, to demonstrate it we're going to assume the answer and prove that its path integral corresponds to Eq.(8)

QUENCHED CANONICAL DENSITY MATRIX

To proceed, we're going to postulate what we term a quenched canonical density matrix

$$\bar{\rho}(\hbar\beta) = \frac{1}{Z_\beta}\hat{\tau} \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \;\bar{H}(\tau)\right] \tag{11}$$

I'm not sure if this object already exists in the literature, but I've not encountered it in an (admittedly cursory) survey. Physically, it should probably be interpreted as the equilibrium density matrix produced from a temperature dependent Hamiltonian, when one quenches from infinite temperature, down to the desired temperature. The $\hat{\tau}$ operator orders inverse-temperatures, in much the same way as the time ordering operator does for real time propagators. We shall now demonstrate that the path integral representation of this density matrix has the form of the imaginary time path integral of the previous section.

The quenched density in coordinate space is:

$$\bar{\rho}(q;q') = \langle q|\bar{\rho}|q'\rangle \tag{12}$$

In order to generate the path integral, we must first discretise the operator using $\Delta N = \hbar\beta$ and $\bar{H}_j = \bar{H}(j\Delta)$:

$$\exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau\ \bar{H}(\tau)\right] \to \exp\left[-\frac{1}{\hbar}\sum_{j=0}^{N}\Delta\bar{H}_j\right]. \tag{13}$$

We know that we will take the limit $\Delta \to 0$ to obtain the path integral, so we will apply the Zassenhaus approximation to our discretised density. This approximation states

$$\exp\left[\Delta\left(\hat{A}+\hat{B}\right)\right] = \exp\left[\Delta\hat{A}\right]\exp\left[\Delta\hat{B}\right]\exp\left[-\frac{\Delta^2}{2}\left[\hat{A},\hat{B}\right]_-\right] \times \mathcal{O}\left(\Delta^3\right) \tag{14}$$

which after application yields

$$Z\bar{\rho} \approx \left[\prod_{j=0}^{N-1}\exp\left[-\frac{\Delta^2}{2\hbar^2}\left[\bar{H}_{j+1},\bar{H}_j\right]_-\right]\right]\hat{\tau}\prod_{j=0}^{N}\exp\left[-\frac{1}{\hbar}\Delta\bar{H}_j\right]. \tag{15}$$

If we assume the commutator between any two of $\bar{H}_j$ is proportional to $\hbar$ then we have

$$\left[\prod_{j=0}^{N-1}\exp\left[-\frac{\Delta^2}{2\hbar^2}\left[\bar{H}_{j+1},\bar{H}_j\right]_-\right]\right] \propto \exp\left[-\frac{a\Delta^2}{2\hbar}\right]. \tag{16}$$

In the limit this term will become unity, so we shall neglect it and focus on the remaining part $\hat{\tau}\prod_{j=0}^{N}\exp\left[-\frac{1}{\hbar}\Delta\bar{H}_j\right]$. After τ ordering this the term becomes

$$\hat{\tau}\prod_{j=0}^{N}\exp\left[-\frac{1}{\hbar}\Delta\bar{H}_j\right] = \exp\left[-\frac{1}{\hbar}\Delta\bar{H}_N\right]...\exp\left[-\frac{1}{\hbar}\Delta\bar{H}_j\right]...\exp\left[-\frac{1}{\hbar}\Delta\bar{H}_0\right]. \tag{17}$$

We can use the Zassenhaus approximation again to split the Hamiltonian into its kinetic and potential parts

$$Z_\beta\bar{\rho}(q;q') \approx \langle q|\exp\left[-\frac{1}{\hbar}\Delta\bar{T}_N\right]\exp\left[-\frac{1}{\hbar}\Delta\bar{V}_N\right]...\exp\left[-\frac{1}{\hbar}\Delta\bar{T}_0\right]\exp\left[-\frac{1}{\hbar}\Delta\bar{V}_0\right]|q'\rangle. \tag{18}$$

Now we insert a resolution of the identity in terms of the $\bar{V}_j$ position eigenstates. This gives:

$$\bar{\rho}(q;q') = \int \mathrm{d}q_1...\mathrm{d}q_n\prod_{j=0}^{N}\left\langle q_{j+1}\left|\exp\left[-\frac{1}{\hbar}\Delta\bar{T}_j\right]\exp\left[-\frac{1}{\hbar}\Delta\bar{V}_j\right]\right|q_j\right\rangle \tag{19}$$

using $|q_0\rangle = |q'\rangle$ and $|q_{N+1}\rangle = |q\rangle$.

We are now in a position to evaluate a single term in the product

$$\left\langle q_{j+1} \left| \exp\left[-\frac{1}{\hbar}\Delta\bar{T}_j\right] \exp\left[-\frac{1}{\hbar}\Delta\bar{V}_j\right] \right| q_j \right\rangle = \left\langle q_{j+1} \left| \exp\left[-\frac{1}{\hbar}\Delta\bar{T}_j\right] \right| q_j \right\rangle \exp\left[-\frac{1}{\hbar}\Delta\bar{V}(q_j, j\Delta)\right] \tag{20}$$

while the kinetic operator can be assessed by transforming to the momentum basis

$$\left\langle q_{j+1} \left| \exp\left[-\frac{1}{\hbar}\Delta\bar{T}_j\right] \right| q_j \right\rangle = \int dp \; \langle q_{j+1}| \exp\left[-\frac{1}{\hbar}\Delta\bar{T}_j\right] |p\rangle\langle q_j|p\rangle \tag{21}$$

$$= \int dp \; \langle q_{j+1}|p\rangle\langle q_j|p\rangle \exp\left[-\frac{\Delta p^2}{2m\hbar}\right] \tag{22}$$

resulting in the following expression for a single term:

$$\left\langle q_{j+1} \left| \exp\left[-\frac{1}{\hbar}\Delta\bar{T}_j\right] \exp\left[-\frac{1}{\hbar}\Delta\bar{V}_j\right] \right| q_j \right\rangle = \int dp \; \frac{1}{2\pi\hbar} \exp\left[-\frac{1}{\hbar}\left(\frac{\Delta p^2}{2m} - i\left(q_{j+1} - q_j\right)\right)\right]. \tag{23}$$

This can be integrated by completing the square

$$\left\langle q_{j+1} \left| \exp\left[-\frac{1}{\hbar}\Delta\bar{T}_j\right] \right| q_j \right\rangle = \sqrt{\frac{m}{2\pi\hbar\Delta}} \exp\left[-\frac{m}{2\Delta\hbar}\left(q_{j+1} - q_j\right)^2\right] \tag{24}$$

and reinserted into Eq.(19) to produce the path integral representation for the quenched density:

$$\bar{\rho}(q; q') = \lim_{\Delta\to 0} \frac{1}{Z_\beta} \int \prod_{j=0}^{N} \left(\sqrt{\frac{\mathrm{m}}{2\pi\hbar\Delta}} \mathrm{d}q_j\right) \exp\left[-\frac{\Delta}{\hbar}\left(\frac{m\left(q_{j+1} - q_j\right)^2}{2\Delta^2} + \bar{V}(q_j, j\Delta)\right)\right] \tag{25}$$

$$= \frac{1}{Z_\beta} \int \mathcal{D}\bar{q}(\tau) \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \; \bar{H}(\tau)\right] \tag{26}$$

with $\bar{H}(\tau)$ being a simple function of imaginary time (not an operator).

The path integral representation of the initial density matrix in Eq. (8) may now be identified with Eq. (11), using an effective Hamiltonian given by Eq. (9). We further specify however that neither the Hamiltonian or its coupling have any temperature dependence (i.e. only the noise is a function of imaginary time):

$$\overline{H}\left(\tau\right) = \hat{H}_Q + \bar{\mu}\left(\tau\right)\hat{f}. \tag{27}$$

The initial (stochastic) reduced density operator is now characterised as a propagator through imaginary time:

$$\widetilde{\rho}_0 \equiv \overline{\rho}(\tau)\big|_{\tau=\beta\hbar} \tag{28}$$

using

$$\overline{\rho}(\tau) = \frac{1}{Z_\beta}\hat{\tau}\exp\left[-\frac{1}{\hbar}\int_0^\tau \mathrm{d}\tau' \ \left(\hat{H}_Q + \bar{\mu}\left(\tau'\right)\hat{f}\right)\right]. \tag{29}$$

This density operator $\overline{\rho}(\tau)$ is responsible for the thermalisation of the open system (when $\tau \to \beta\hbar$) and satisfies the Schrödinger-like equation of motion:

$$-\hbar\partial_\tau\overline{\rho}(\tau) = \overline{H}(\tau)\overline{\rho}(\tau) \tag{30}$$

$$\overline{\rho}(\tau = 0) = Z_\beta^{-1} \tag{31}$$

Note that the partition function should only depend on the final temperature. Practically, one would perform this the evolution with the initial condition $\overline{\rho}(\tau = 0) = \mathbb{1}$, and normalising at the end of the evolution $\mathrm{Tr}_Q\left[\overline{\rho}(\beta\hbar)\right] = 1$ to fix Z_β.

The Hamiltonian H_Q and the interaction operators in $\overline{H}(\tau)$ have no temperature dependence, but instead the temperature sets the propagation "time" $\tau = \beta\hbar$. This hard limit relating the time to the system temperature is important, as unlike in the real time case, the effective initial density matrix may diverge as we take $\tau \to \infty$. This is a reflection of the fact that the path integral description of the canonical density matrix is itself only defined for finite temperature.

HAMILTONIAN OF MEAN FORCE

So, with this setup, let's get to the Hamiltonian of mean force. The imaginary time differential equation allows for the exact calculation of the *reduced equilibrium density matrix*. This is important, as the stationary distribution of dissipative systems with finite couplings has been shown to deviate from that expected under partitioned conditions [3]. Describing the statistics of such a system is not trivial, necessitating a formulation of thermodynamic laws beyond the assumption of weak environmental coupling [4]. This is sometimes achieved by defining a "Hamiltonian of mean force" $\hat{H}_{MF}$. This is the effective Hamiltonian that describes the canonical distribution of the open system after tracing out the bath:

$$\hat{H}_{MF} = -\frac{1}{\beta} \ln \left(\frac{\mathrm{Tr}_X \left[\mathrm{e}^{-\beta \hat{H}_{\mathrm{tot}}} \right]}{\mathrm{Tr}_X \left[\mathrm{e}^{-\beta \hat{H}_{\mathrm{X}}} \right]} \right) \tag{32}$$

such that the reduced system in equilibrium is described by

$$\rho_0 = \frac{1}{Z_\beta} \mathrm{e}^{-\beta \hat{H}_{MF}}. \tag{33}$$

where Z_β is defined in the same way as previously- Clearly $\hat{H}_{MF}$ is closely related to the reduced canonical density given in Eq.(29). Using this, it is possible to approximate the Hamiltonian of mean force for a CL environment. To do so we start from the reduced density operator

$$\widetilde{\rho}_0 = \hat{\tau} \exp \left[-\beta \hat{H}_Q - \frac{1}{\hbar} \hat{f} \int_0^{\beta\hbar} \mathrm{d}\tau \ \bar{\mu}(\tau) \right]. \tag{34}$$

Note I'm ignoring the partition function as it is by definition the one corresponding to that defined for the Hamiltonian of mean force. I'll therefore set it to 1 as it's irrelevant to the argument. Upon averaging and normalising, the reduced density operator will give the physical initial reduced density matrix in Eq. (33) and hence a way to assign $\hat{H}_{MF}$. As a first approximation we express $\tilde{\rho}_0$ as

$$\widetilde{\rho}_0 \approx \mathrm{e}^{-\beta \hat{H}_Q} \hat{\tau} \exp \left[-\frac{1}{\hbar} \hat{f} \int_0^{\beta\hbar} \mathrm{d}\tau \ \bar{\mu}(\tau) \right]. \tag{35}$$

This will obviously be exact when the system and interaction commute (say for example a two level system where both $\hat{H}_Q$ and $\hat{f}$ are both proporional to σ_z), but problematically this is an uncontrolled approximation [5] when $\left[\hat{H}_Q, \hat{f} \right]_- \neq 0$. One can work around this if an explicit form for $\hat{f}$ is given, but even with this approximation we are at least able to draw out some important characteristics of the Hamiltonian of mean force - namely that it depends on both temperature and the *square* of the system-environment coupling.

To evaluate the average, we first expand the stochastic exponential

$$\hat{\tau} \exp \left[-\frac{1}{\hbar} \hat{f} \int_0^{\beta\hbar} \mathrm{d}\tau \ \bar{\mu}(\tau) \right] = \sum_n \frac{1}{n!} \left(-\frac{1}{\hbar} \hat{f} \int_0^{\beta\hbar} \mathrm{d}\tau \ \bar{\mu}(\tau) \right)^n. \tag{36}$$

Any term with an odd power of $\hat{f}$ in this expansion can be discarded, since from Isserlis'/Wick's theorem [6] the average over an odd product of zero-mean Gaussian noises is zero:

$$\left\langle \exp \left[-\frac{1}{\hbar} \hat{f} \int_0^{\beta\hbar} \mathrm{d}\tau \ \bar{\mu}(\tau) \right] \right\rangle_r = \sum_n \frac{1}{(2n)!} \left\langle \left(-\frac{1}{\hbar} \hat{f} \int_0^{\beta\hbar} \mathrm{d}\tau \ \bar{\mu}(\tau) \right)^{2n} \right\rangle_r. \tag{37}$$

Wick's theorem can also be used to assess this average when n is even

$$\left\langle \left(\int \mathrm{d}\tau \bar{\mu}\left(\tau\right) \right)^{2n} \right\rangle_r = \frac{(2n)!}{2^n n!} C\left(\beta\right)^n \tag{38}$$

$$C\left(\beta\right) = \int \mathrm{d}\tau \mathrm{d}\tau' \ \left\langle \bar{\mu}\left(\tau\right) \bar{\mu}\left(\tau'\right) \right\rangle_r . \tag{39}$$

Note that $C(\beta)$ is completely specified when $I(\omega)$ is provided. Substituting this into the series expansion yields:

$$\sum_n \frac{1}{(2n)!} \left\langle \left(-\frac{1}{\hbar} \hat{f} \int_0^{\beta\hbar} \mathrm{d}\tau \ \bar{\mu}\left(\tau\right) \right)^{2n} \right\rangle_r = \sum_n \frac{1}{2^n n!} \left(-\frac{1}{\hbar} \hat{f} \right)^{2n} C\left(\beta\right)^n \tag{40}$$

$$\implies \left\langle \exp\left[-\frac{1}{\hbar} \hat{f} \int_0^{\beta\hbar} \mathrm{d}\tau \ \bar{\mu}\left(\tau\right) \right] \right\rangle_r = \exp\left[\frac{1}{2\hbar^2} \hat{f}^2 C\left(\beta\right) \right] \tag{41}$$

which can be used to give a first approximation to the Hamiltonian of mean force for CL models

$$\hat{H}_{MF} \approx \hat{H}_Q - \frac{1}{2\beta\hbar^2} \hat{f}^2 C\left(\beta\right) . \tag{42}$$

As promised, this approximation captures at least the first order effect of the environment coupling. Another important point to note here is that this extra contribution *only* occurs when the noise is quantum. A very heuristic way to see this is $\lim_{\hbar\to 0} \left\langle \bar{\mu}\left(\tau\right) \bar{\mu}\left(\tau'\right) \right\rangle_r = 0$, meaning the noise becomes totally uncorrelated and can be neglected from the dynamics. A slightly more sophisticated argument is to construct the classical path integral via Koopman von-Neumann dynamics for the joint system. While the real time propagator has a similar influence functional structure, the imaginary time evolution is redundant, and the thermal state can always be treated as non-interacting with the addition of a counter-term to the system Hamiltonian. See Ref. [7] for a more complete explanation of this phenomenon.

NOISE AVERAGING AND EFFECTIVE HAMILTONIAN VIA THE INTERACTION PICTURE

We consider a quantum system subject to stochastic perturbations, modeled by a Hamiltonian of the form

$$H(\tau) = H_Q + \mu(\tau) f, \tag{43}$$

where H_Q is the deterministic system Hamiltonian, f is a Hermitian operator coupling to the noise, and $\mu(\tau)$ is a zero-mean Gaussian stochastic process with correlation function

$$K(\tau - \tau') = \mathbb{E}[\mu(\tau)\mu(\tau')]. \tag{44}$$

We work in imaginary time $\tau \in [0, \beta\hbar]$.

Our object of interest is the noise-averaged thermal density matrix

$$\rho = \mathbb{E}\left[\mathcal{T} \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau' \left(H_Q + \mu(\tau')f\right)\right)\right], \tag{45}$$

where $\mathcal{T}$ denotes imaginary-time ordering.

Interaction Picture Transformation

We move to the interaction picture with respect to H_Q, defining

$$U(\tau) = e^{-\frac{\tau}{\hbar}H_Q}V(\tau). \tag{46}$$

In this frame, $V(\tau)$ satisfies

$$\frac{dV}{d\tau} = -\frac{1}{\hbar}\mu(\tau)\tilde{f}(\tau)V(\tau), \qquad \tilde{f}(\tau) = e^{\frac{\tau}{\hbar}H_Q} f e^{-\frac{\tau}{\hbar}H_Q}. \tag{47}$$

Thus, formally,

$$V(\beta\hbar) = \mathcal{T} \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau' \mu(\tau')\tilde{f}(\tau')\right). \tag{48}$$

Substituting back, the full density matrix becomes

$$\rho = e^{-\beta H_Q}\mathbb{E}\left[\mathcal{T} \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau' \mu(\tau')\tilde{f}(\tau')\right)\right]. \tag{49}$$

Stochastic Averaging

Since $\mu(\tau)$ is Gaussian and zero mean, the noise average reduces to a cumulant expansion:

$$\mathbb{E}\left[\mathcal{T} e^{\int d\tau X(\tau)}\right] = \mathcal{T} \exp\left(\frac{1}{2}\int d\tau d\tau' \langle X(\tau)X(\tau')\rangle\right) \tag{50}$$

for any linear functional $X(\tau)$ of $\mu(\tau)$. Applying this with $X(\tau) = -\mu(\tau)\tilde{f}(\tau)/\hbar$, we find

$$\rho = e^{-\beta H_Q}\mathcal{T} \exp\left(\frac{1}{2\hbar^2}\int_0^{\beta\hbar} d\tau d\tau' K(\tau - \tau')\tilde{f}(\tau)\tilde{f}(\tau')\right). \tag{51}$$

Expansion of $\tilde{f}(\tau)$f(tau)

We expand $\tilde{f}(\tau)$ using the Baker-Campbell-Hausdorff (BCH) formula:

$$\tilde{f}(\tau) = f + \frac{\tau}{\hbar}[H_Q, f] + \frac{1}{2!}\left(\frac{\tau}{\hbar}\right)^2 [H_Q, [H_Q, f]] + \cdots . \tag{52}$$

Substituting into $\tilde{f}(\tau)\tilde{f}(\tau')$ and expanding systematically yields:

$$\tilde{f}(\tau)\tilde{f}(\tau') = f^2 + \frac{1}{\hbar}\left(\tau[H_Q, f]f + \tau' f[H_Q, f]\right) \tag{53}$$

$$+ \frac{1}{\hbar^2}\left(\frac{\tau^2}{2}[H_Q, [H_Q, f]]f + \frac{\tau'^2}{2} f[H_Q, [H_Q, f]] + \tau\tau'[H_Q, f][H_Q, f]\right) + \cdots . \tag{54}$$

Effective Hamiltonian

Inserting the expansion back into the double integral, and using the symmetry of $K(\tau - \tau')$, the first-order terms vanish. To second order, we define:

$$C_0 = \int_0^{\beta\hbar} d\tau d\tau' K(\tau - \tau'), \tag{55}$$

$$C_{2a} = \int_0^{\beta\hbar} d\tau d\tau' K(\tau - \tau')\tau^2, \tag{56}$$

$$C_{2c} = \int_0^{\beta\hbar} d\tau d\tau' K(\tau - \tau')\tau\tau'. \tag{57}$$

The correction exponent then becomes

$$\Delta = \frac{C_0}{2\hbar^2} f^2 + \frac{C_{2a}}{4\hbar^4}\{[H_Q, [H_Q, f]], f\} + \frac{C_{2c}}{2\hbar^4}[H_Q, f]^2 + \cdots , \tag{58}$$

where $\{\cdot, \cdot\}$ denotes the anticommutator.

To leading order, we identify the mean-force Hamiltonian H_{MF} via

$$\rho \approx e^{-\beta H_{\mathrm{MF}}}, \qquad H_{\mathrm{MF}} = H_Q - \frac{1}{\beta}\Delta. \tag{59}$$

Classical Limit

In the classical limit $\hbar \to 0$, commutators scale as

$$[A, B] \sim i\hbar\{A, B\}_{\mathrm{PB}}, \tag{60}$$

where $\{A, B\}_{\mathrm{PB}}$ denotes the Poisson bracket. Thus:

$$[H_Q, f] \to i\hbar\{H_Q, f\}_{\mathrm{PB}}, \tag{61}$$

$$[H_Q, [H_Q, f]] \to -(\hbar^2)\{H_Q, \{H_Q, f\}_{\mathrm{PB}}\}_{\mathrm{PB}}. \tag{62}$$

Substituting these scalings into Δ shows that all terms involving commutators scale uniformly with $\hbar^{-2}$.

Furthermore, the f^2 term, initially appearing with a $\hbar^{-2}$ prefactor, sees its coefficient C_0 scale as $C_0 \sim (\beta\hbar)^2$, canceling the $\hbar$ dependence. Thus, the static noise-induced potential survives the classical limit.

Summary

In the classical limit, the mean-force Hamiltonian becomes

$$\begin{aligned} H_{\mathrm{MF}}^{\mathrm{classical}} = H_Q &- \frac{1}{\beta}\left(\frac{\beta^2}{2}K(0)f^2\right) \\ &- \frac{1}{\beta}\left(-\frac{C_{2a}}{4}\{\{H_Q, \{H_Q, f\}_{\mathrm{PB}}\}_{\mathrm{PB}}, f\} - \frac{C_{2c}}{2}\{H_Q, f\}_{\mathrm{PB}}^2\right) + \cdots . \end{aligned} \tag{63}$$

Noise corrections thus persist in the classical limit, modifying both the effective potential landscape and the structure of classical phase-space flows.

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