Density Matrix Theory

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Sheet 10

1. Extremal paths

Consider a quantum system defined by the Hamiltonian

$$H_{\rm S} = \frac{P^2}{2M} + V(Q)$$

where Q is a generalized coordinate and P is the momentum canonically conjugated of Q. If the system is coupled to a set of harmonic oscillators in thermal equilibrium, it is possible to express the evolution of the reduced density matrix for the system, in the position representation, in presence of the bath via the the formula:

$$\rho_{red}(Q_f, Q'_f, t) = \int \mathrm{d}Q_i \int \mathrm{d}Q'_i \;\; \rho_{\rm S}(Q_i, Q'_i, 0) J_{\rm FV}(Q_f Q'_f t, Q_i Q'_i 0)$$

where $\rho_{\rm S}(Q_i, Q'_i, 0)$ is the density matrix for the system at time $t = 0$ and the propagating function $J_{\rm FV}$ reads

$$J_{\rm FV} = \int \mathcal{D}Q \int \mathcal{D}Q' \;\; \mathcal{A}[Q]\mathcal{A}^*[Q']\mathcal{F}_{\rm FV}[Q, Q'; t].$$

In this last formula $\mathcal{A}[\mathcal{Q}]$ stands for the propagator of the isolated system calculated along the path $Q(t)$, while $\mathcal{F}_{\rm FV}[Q, Q'; t]$ is the Feynman-Vernon influence functional. If the system is coupled to the bath linearly in the bath coordinates, the influence functional can be written as:

$$\mathcal{F}_{\rm FV}[Q, Q'; t] = \exp(-\Phi_{\rm FV}[\eta, \xi])$$

where

$$\Phi_{\rm FV}[\eta,\zeta] = \frac{1}{\hbar^2}\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t''[\zeta(t')R(t'-t'')\zeta(t'') + i2\zeta(t')I(t'-t'')\eta(t'')] + \frac{iM\gamma(0^+)}{\hbar}\int_0^t \mathrm{d}t'\zeta(t')\eta(t')$$

and in the latter we have used the real and imaginary parts of the force-force correlator $\langle F(t)F(t')\rangle = R(t-t') + iI(t-t')$ and also the dissipative kernel $\gamma(t)$. We have also introduced the center of mass and relative coordinates η and ζ respectively, defined as:

$$\eta(\tau) = \frac{1}{2}[Q(\tau) + Q'(\tau)]$$
$$\zeta(\tau) = Q(\tau) - Q'(\tau)$$

1. Verify that the propagating function $J_{\rm FV}$ contains both a contribution local and non-local in time and prove that it can be cast into the form:

$$J_{\rm FV} = \int \mathcal{D}\eta \int \mathcal{D}\zeta \, \mathrm{e}^{\frac{i}{\hbar}S_{\rm L}[\eta,\zeta]}\mathrm{e}^{\frac{i}{\hbar}S_{\rm NL}[\eta,\zeta]}$$

where the local contribution to the action $S_{\mathrm{L}}[\eta,\zeta]$ reads

$$S_{\mathrm{L}}[\eta,\zeta] = \int_0^t \mathrm{d}t'[M\dot{\eta}\dot{\zeta} + V(\eta-\zeta/2) - V(\eta+\zeta/2) - M\gamma(0)\zeta(t')\eta(t')]$$

while the non-local contribution $S_{\mathrm{NL}}[\eta,\zeta]$ reads

$$S_{\mathrm{NL}}[\eta,\zeta] = \frac{i}{\hbar}\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t''[\zeta(t')R(t'-t'')\zeta(t'') + i2\zeta(t')I(t'-t'')\eta(t'')]$$

2. Prove the paths that minimize the action $S = S_{\mathrm{L}} + S_{\mathrm{NL}}$ are solutions of the coupled integro-differential equations:

$$\begin{cases} 0 = -M\ddot{\zeta}(s) + \frac{\partial}{\partial\eta}[V(\eta-\zeta/2) - V(\eta+\zeta/2)] - \frac{2}{\hbar}\int_s^t \mathrm{d}t'\zeta(t')I(t'-s) - M\gamma(0)\zeta(s) \\ 0 = -M\ddot{\eta}(s) + \frac{\partial}{\partial\zeta}[V(\eta-\zeta/2) - V(\eta+\zeta/2)] - \frac{2}{\hbar}\int_0^s \mathrm{d}t' I(s-t')\eta(t') - M\gamma(0)\eta(s) \\ \quad + \frac{i}{\hbar}\int_0^t \mathrm{d}t' R(s-t')\zeta(t') \end{cases} \tag{1}$$

Hint you should calculate first δS and set it equal to zero for every variation $\delta\eta$ and $\delta\zeta$ of the independent paths η and ζ. Remember also that for the real part of the force-force correlator $R(t) = R(-t)$.

3. Prove that, according to the result derived at the previous point, in the absence of noise $\zeta \equiv 0$ the variable η satisfies the classical noiseless Langevin equation

$$M\ddot{\eta}(s) + M\int_0^s \mathrm{d}t'\, \gamma(s-t')\dot{\eta}(t') + M\gamma(s)\eta(0) + \frac{\mathrm{d}}{\mathrm{d}\eta}V(\eta) = 0$$

Hint: it is useful to remember the relation connecting the imaginary component of the force-force correlator to the dissipative kernel: $I(t) = \hbar\frac{M}{2}\frac{\mathrm{d}}{\mathrm{d}t}\gamma(t)$

4. Now calculate the semiclassical limit obtained by reintroducing the fluctuations ζ, but just to the second order (Gaussian fluctuations). Prove that the result is

$$\begin{cases} \ddot{\eta}(s) + \frac{\mathrm{d}}{\mathrm{d}s}\int_0^s \mathrm{d}t'\, \gamma(s-t')\eta(t') + \frac{1}{M}\frac{\mathrm{d}}{\mathrm{d}\eta}V(\eta) = \frac{i}{\hbar M}\int_0^t \mathrm{d}t' R(s-t')\zeta(t') \\ \ddot{\zeta}(s) - \frac{\mathrm{d}}{\mathrm{d}s}\int_s^t \mathrm{d}t'\gamma(t'-s)\zeta(t') + \frac{1}{M}\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}V(\eta)\zeta = 0 \end{cases} \tag{2}$$

5. Specialize the result obtained at the previous point to the case of an harmonic oscillator $V(Q) = \frac{1}{2}M\omega_0^2 Q^2$. The Gaussian approximation is exact in this case, why?

Frohes Schaffen!