Density Matrix Theory

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Sheet 11

1. The quasiclassical action of a damped harmonic oscillator (DHO)

Let us consider, as in the question 1.5 of Sheet 10 a harmonic oscillator with potential $V(Q) = \frac{1}{2}M\omega_0^2 Q^2$ interacting with a heat bath described by the force-force correlator $\langle \hat{F}(t)\hat{F}(0)\rangle_{\rm B} = R(t) + iI(t)$. The propagating function is then written in the form:

$$J_{\rm FV}(\eta_f, \zeta_f, t; \eta_i, \zeta_i, 0) = \int \mathcal{D}\eta \mathcal{D}\zeta \, e^{\frac{i}{\hbar}S[\eta,\zeta]} \tag{1}$$

where the path integral is extended to all the paths η and ζ satisfying the boundary conditions

$$\begin{cases} \eta_f = \eta(t) \\ \zeta_f = \zeta(t) \end{cases} \quad \text{and} \quad \begin{cases} \eta_i = \eta(0) \\ \zeta_i = \zeta(0) \end{cases} \tag{2}$$

The action S was analyzed in detail in Sheet 10 as the combination of a time local and time non local contributions

$$S = S_{\rm L} + S_{\rm NL}. \tag{3}$$

Moreover, let us define the paths η_{cl} and ζ_{cl} as the ones that minimize the action S. They are defined (in the harmonic oscillator case considered here) by the equations:

$$\begin{cases} \ddot{\eta}(s) + \frac{\rm d}{{\rm d}s}\int_0^s {\rm d}t'\, \gamma(s-t')\eta(t') + \omega_0^2\eta = \frac{i}{\hbar M}\int_0^t {\rm d}t' R(s-t')\zeta(t') \\ \ddot{\zeta}(s) - \frac{\rm d}{{\rm d}s}\int_s^t {\rm d}t' \gamma(t'-s)\zeta(t') + \omega_0^2\zeta = 0 \end{cases} \tag{4}$$

1. Show that, when evaluated on the classical paths, the action S can be casted into the form:

$$S[\eta_{cl}, \zeta_{cl}] = M(\dot{\eta}_f\zeta_f - \dot{\eta}_i\zeta_i) - \frac{i}{2\hbar}\int_0^t {\rm d}s \int_0^t {\rm d}t' \zeta_{cl}(s)R(s-t')\zeta_{cl}(t') \tag{5}$$

2. The boundary values of the paths are real by construction. Nevertheless, due to the imaginary kernel that mixes in the equation (4), the classical path η_{cl} cannot be taken as real. The path ζ_{cl} is instead real (why?). We introduce the notation $\eta_{cl} = \eta_{cl}^{(1)} + i\eta_{cl}^{(2)}$ to distinguish the real and imaginary components. It follows that $\eta_{cl}^{(2)}$ is the solution of:

$$\ddot{\eta}_{cl}^{(2)}(s) + \omega_0^2\eta_{cl}^{(2)}(s) + \frac{\rm d}{{\rm d}s}\int_0^s {\rm d}t' \gamma(s-t')\eta_{cl}^{(2)}(t') = \frac{1}{M\hbar}\int_0^t {\rm d}t' R(s-t')\zeta_{cl}(t') \tag{6}$$

Show, using (5), that the classical action can be expressed in terms of $\eta_{cl}^{(1)}$ only, i.e.:

$$S[\eta_{cl}, \zeta_{cl}] = S^*[\eta_{cl}^{(1)}, \zeta_{cl}] = M(\dot{\eta}_f^{(1)}\zeta_f - \dot{\eta}_i^{(1)}\zeta_i) + \frac{i}{2\hbar}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s' \zeta_{cl}(s) R(s-s') \zeta_{cl}(s'). \quad (7)$$

Hint: to prove (7) first show that

$$\frac{i}{\hbar}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s' \zeta_{cl}(s) R(s-s') \zeta_{cl}(s') = iM(\dot{\eta}_f^{(2)}\zeta_f - \dot{\eta}_i^{(2)}\zeta_i).$$

2. The propagating function of a DHO

The propagating function can be calculated starting from the quasiclassical action obtained in the previous point by accounting for the quantum fluctuations about the classical paths. Due to the form of the system hamiltonian, the quantum fluctuations only enter the normalization factor and the propagating function takes the form:

$$J_{\mathrm{FV}}(\eta_f, \zeta_f, t; \eta_i, \zeta_i, 0) = e^{\frac{i}{\hbar}S[\eta_{cl}, \zeta_{cl}]} N(t, 0)$$

The prefactor $N(t, 0)$ can be calculated by exploiting that, due to conservation of probability, is:

$$\int \mathrm{d}Q_f \; \rho_{red}(Q_f, Q_f, t) = 1. \quad (8)$$

To this extent:

1. Show that:

$$\int \mathrm{d}\eta_f J_{FV}(\eta_f, \zeta_f = 0, t; \eta_i, \zeta_i, 0) = \delta(\zeta_i) \quad (9)$$

   where δ indicates the Dirac delta.

   Hint: Use the definition of J_{FV} in terms of total system propagators, the factorizability of the initial density matrix and the fact that $\mathrm{Tr}\{\rho\} = 1$ for a generic density matrix ρ if the trace is taken over the entire Hilbert space where ρ is defined.

2. Using (9) demonstrate that:

$$N(t, 0) = \frac{M}{2\pi\hbar|G_2(t)|} \quad (10)$$

   where, as discussed in the lecture, $G_2(t)$ is one of the fundamental solutions of the classical Langevin equation for the DHO. In particular, its Laplace transform reads:

$$\tilde{G}_2(z) = \frac{1}{z^2 + \tilde{\gamma}(z)z + \omega_0^2}$$

   where $\tilde{\gamma}$ is the Laplace transform of the damping kernel.

Frohes Schaffen!