Density Matrix Theory

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Sheet 12

1. Damped harmonic oscillator: expectation values of $\hat{Q}$ and $\hat{P}$

Consider a harmonic oscillator of frequency ω_0 and mass M linearly coupled to a dissipative bath with the force-force correlation function $\langle F(t)F(0)\rangle_{\rm B} = R(t) + iI(t)$. Using the exact Feynmann-Vernon propagator calculated in the Sheet 10 you will obtain here the time evolution of the expectation values of position and momentum operators.

1. As a preliminary task prove that the expectation value of the position and momentum operators for a generic system described by the density operator $\hat{\rho}$ can be cast into the form:

$$\begin{cases} \langle \hat{Q} \rangle_t = \int {\rm d}\eta {\rm d}\zeta \; \delta(\zeta)\eta\, \rho(\eta,\zeta,t) \\ \\ \langle \hat{P} \rangle_t = \int {\rm d}\eta {\rm d}\zeta \; \delta(\zeta)\left(\frac{\hbar}{i}\frac{\partial}{\partial\zeta}\right)\rho(\eta,\zeta,t) \end{cases} \tag{1}$$

   where $\eta = (Q+Q')/2$ and $\zeta = Q'-Q$ are the center of mass and relative position, respectively, and they are written in terms of the positions Q and Q' which define the density operator in the position representation: $\rho(Q,Q',t) \equiv \langle Q|\hat{\rho}|Q'\rangle$.

   Hint: Make use of the completeness relations for the position and momentum eigenstates:

$$\mathbf{1} = \int {\rm d}Q |Q\rangle\langle Q| \qquad \text{and} \qquad \mathbf{1} = \int {\rm d}P \frac{1}{2\pi\hbar}|P\rangle\langle P|$$

   .

2. The density matrix at time t, $\rho(\eta_f,\zeta_f,t)$, can be written in terms of the initial density matrix and the propagator $J_{\rm FV}$ according to the formula:

$$\rho(\eta_f,\zeta_f,t) = \int {\rm d}\eta_{\rm i}{\rm d}\zeta_{\rm i}\; J_{\rm FV}(\eta_f,\zeta_f,t;\eta_i,\zeta_i,0)\rho(\eta_i,\zeta_i,0). \tag{2}$$

   In the Sheet 11 you have already expressed the propagator as a function of the classical action S and the normalization function N: $J_{\rm FV} = Ne^{\frac{i}{\hbar}S[\eta_{cl},\zeta_{cl}]}$.

   Find the explicit form of J_{FV} as a function of η_i, ζ_i, η_f, ζ_f and t. In particular prove that, for the classical action, it holds:

$$S[\eta_{cl},\zeta_{cl}] = M\sum_{\alpha\beta}\left(\eta_\alpha\Gamma^{(1)}_{\alpha\beta}\zeta_\beta + i\zeta_\alpha\Gamma^{(2)}_{\alpha\beta}\zeta_\beta\right)$$

   where α, $\beta = i, f$ and the matrices $\mathbf{\Gamma}^{(1)}$ and $\mathbf{\Gamma}^{(2)}$ are functions of the time only.

Prove in fact that the elements of $\mathbf{\Gamma}^{(1)}$ read:

$$\Gamma^{(1)}_{ii} = \Gamma^{(1)}_{ff} = \frac{\dot{G}_2(t)}{G_2(t)}, \qquad \Gamma^{(1)}_{fi} = -\frac{1}{G_2(t)} \quad \text{and} \quad \Gamma^{(1)}_{if} = \ddot{G}_2(t) - \frac{[\dot{G}_2(t)]^2}{G_2(t)}, \tag{3}$$

where $G_2(t)$ is the inverse Laplace transform of $\tilde{G}_2(z) = [z^2 + z\tilde{\gamma}(z) + \omega_0^2]^{-1}$ and $\gamma(t)$ is related to the imaginary part of the force-force correlator by the relation $I(t) = \frac{\hbar M}{2}\frac{\mathrm{d}}{\mathrm{d}t}\gamma(t)$.

Moreover prove that the elements of $\mathbf{\Gamma}^{(2)}$ read:

$$\begin{aligned}
\Gamma^{(2)}_{ii} &= \frac{1}{2M\hbar}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s' \; \frac{G_2(t-s)}{G_2(t)} R(s-s') \frac{G_2(t-s')}{G_2(t)}, \\
\Gamma^{(2)}_{if} = \Gamma^{(2)}_{fi} &= \frac{1}{2M\hbar}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s' \; \frac{G_2(t-s)}{G_2(t)} R(s-s') \left[\dot{G}_2(t-s') - \frac{\dot{G}_2(t)}{G_2(t)} G_2(t-s')\right], \\
\Gamma^{(2)}_{ff} &= \frac{1}{2M\hbar}\int_0^t \mathrm{d}s \int_0^t \mathrm{d}s' \; \left[\dot{G}_2(t-s) - \frac{\dot{G}_2(t)}{G_2(t)} G_2(t-s)\right] R(s-s') \left[\dot{G}_2(t-s') - \frac{\dot{G}_2(t)}{G_2(t)} G_2(t-s')\right].
\end{aligned} \tag{4}$$

The normalization factor reads $N = \frac{M}{2\pi\hbar|G_2(t)|}$ and has been calculated in the Sheet 11.

3. By using the results obtained at the first and second point prove that the expectation values of the position and momentum operators can be cast into the form:

$$\begin{aligned}
\langle \hat{Q} \rangle_t &= \dot{G}_2(t)\langle \hat{Q} \rangle_0 + \tfrac{1}{M} G_2(t) \langle \hat{P} \rangle_0 \\
\langle \hat{P} \rangle_t &= \ddot{G}_2(t) M \langle \hat{Q} \rangle_0 + \dot{G}_2(t) \langle \hat{P} \rangle_0
\end{aligned} \tag{5}$$

4. Using the Ehrenfest theorem prove that it is possible to obtain the relation $\langle \hat{P} \rangle_t = M \frac{\mathrm{d}}{\mathrm{d}t} \langle \hat{Q} \rangle_t$ even in presence of a dissipative environment if the coupling to the dissipative bath only depends on the position of the system.

5. Calculate the time evolution of the expectation values of the position and momentum operator for the case of an Ohmic bath which is characterized by a delta correlated damping kernel $\gamma(t) = \gamma\delta(t)$. Prove in particular that:

$$G_2(t) = \frac{1}{\lambda}\sin(\lambda t)\exp(-\gamma t/2)$$

where $\lambda = \sqrt{\omega_0^2 - \gamma^2/4}$. Plot the expectation values as a trajectory in the phase space.

Frohes Schaffen!