I. Harmonic Oscillator

1) For a harmonic oscillator, show that \( C(t) = \langle x(t) x(0) \rangle \) satisfies \( \ddot{C} + \omega_0^2 C = 0 \).

2) Solve for \( C(t) \) and its Fourier transform \( \tilde{C}(\omega) = \int C(t) e^{i\omega t} dt \).

3) The forced oscillator obeys the equation of motion
\[
 m\ddot{x} + m\omega_0^2 x = f(\omega) e^{-i\omega t}.
\]
Derive the expression for \( \chi(\omega) \) from the above equation.

4) Write the formula for \( K(t) \).

5) Verify \( K(t) = -\beta \dot{C}(t) \) [i.e. \( \chi'' = \frac{B_0}{2} \tilde{C}(\omega) \)].

6) *Verify the Kramers-Kronig relations.

II. The relaxation of rotational motions can be described by the rotational diffusion equation \( \frac{\partial p}{\partial t} = D_R \nabla^2 p \), where \( \nabla^2 \) is the angular part of the Laplacian operator
\[
\nabla^2 = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}.
\]

1) Show that the average orientation \( u(t) = \langle \cos \theta(t) \rangle \) satisfies
\[
\dot{u}(t) = -2D_R u(t).
\]

2) Show that the orientational correlation function is given by
\[
C(t) = \langle \cos \theta(t) \cos \theta(0) \rangle = \frac{1}{3} e^{-2D_R t}.
\]

3) Write down \( K(t), \chi', \) and \( \chi'' \).

4) Calculate the response to a monochromatic force \( F(t) = F_0 \cos \omega_0 t \), which couples to the system according to \( H' = -F(t) \cos \theta(t) \).

5) Calculate the average absorption rate.
(Ref: McQuarrie, p. 398, prob. 17-19)

III. Repeat the steps in Problem I for a damped oscillator described by
\[
m\ddot{x} + m\gamma \dot{x} + m\omega_0^2 x = f(t) + F(t),
\]
where \( f(t) \) is the random force and \( F(t) \) is the external driving force.

1) Show the position correlation function satisfies
\[
m\ddot{C} + m\gamma \dot{C} + m\omega_0^2 C = 0
\]
with the initial condition \( C(0) = (\beta m\omega_0^2)^{-1} \).

2) Derive explicit expressions for \( C(t) \) and its Fourier transform \( \tilde{C}(\omega) \).

3) Show that under the external force the average position \( \bar{x} \) satisfies
\[
\ddot{\bar{x}} + \gamma \dot{\bar{x}} + \omega_0^2 \bar{x} = \frac{F(t)}{m}.
\]

4) Solve \( \chi(\omega) \) from the above equation.

5) Derive \( K(t) \) using the expression for \( \chi(\omega) \) found above.
6) Verify \( K(t) = -\beta \dot{C}(t) \).

IV. *Derivation of quantum response theory (Ref: McQuarrie, Berne, Kubo, Reichl).

1) Define the quantum Liouville operator as \( \mathcal{L}A = \frac{i}{\hbar} [H, A] \). Show that \( \dot{A}(t) = i\mathcal{L}(t)A(t) \) and \( \dot{\rho} = -i\mathcal{L}\rho \), where \( \rho \) is the density matrix and \( A(t) \) is a Heisenberg operator.

2) Given \( H = H_0 - AF(t) \), use perturbation theory to show

\[
\langle A(t) \rangle = \int_{-\infty}^{t} K(t-t')F(t')dt',
\]

where \( K(t-t') = \frac{i}{\hbar} \langle [A(t),A(t')] \rangle \).

3) Show that the classical limit of the quantum commutator is:

\[
i\hbar \{ A, B \} = \{ A, B \},
\]

where \( \{ , \} \) is the Poisson bracket.

4) Show that the classical limit of \( K(t) \) is \( -\beta \dot{C}(t) \).

V. Spectroscopic measurements are expressed as polarization responses. We calculate the response function of a linear harmonic oscillator as an example.

1) The linear response function is defined as

\[
R(t) = \frac{i}{\hbar} \langle 0|\alpha(t)\alpha(0)|0 \rangle = \frac{i}{\hbar} \{ 0|\alpha(t)\alpha(0)|0 \} - \langle 0|\alpha(0)\alpha(t)|0 \rangle,
\]

where the transition dipole is assumed to be linear in coordinate \( \alpha(t) = \alpha_0 x(t) \).

Show \( R(t) = \frac{\sin \omega t}{m\omega} \alpha_0^2 \).

Useful expressions:

\( x(t) = \sqrt{\frac{\hbar}{2m\omega}} (ae^{-i\omega t} + \alpha^\dagger e^{i\omega t}) \), \( \langle 0|\alpha\alpha^\dagger|0 \rangle = 1, \langle 0|\alpha^\dagger\alpha|0 \rangle = 0 \).

2) Show that the same result can be obtained classically by replacing the quantum commutation with the Poisson bracket,

\[
\frac{1}{i\hbar} [\alpha(t),\alpha(0)] \rightarrow \{ \alpha(t),\alpha(0) \} = \frac{\partial \alpha(t)}{\partial x(0)} \frac{\partial \alpha(0)}{\partial p(0)} - \frac{\partial \alpha(t)}{\partial p(0)} \frac{\partial \alpha(0)}{\partial x(0)}
\]

Useful expression: \( x(t) = x(0) \cos \omega t + \frac{p(0)}{m\omega} \sin \omega t \)

3) The non-linear response function is defined as

\[
R(t_1, t_2) = \left( \frac{i}{\hbar} \right)^2 \langle 0|[[\alpha(t_1 + t_2),\alpha(t_1)],\alpha(0)]|0 \rangle,
\]

If \( \alpha = \alpha_0 x \), show \( R(t_1, t_2) = 0 \) from the balance of \( \alpha \) and \( \alpha^\dagger \) operators.

4) *To obtain non-vanishing non-linear response for the harmonic oscillator, we introduce a non-linear coordinate dependence,

\( \alpha = \alpha_0 x + \alpha' x^2 + \cdots \)

Show that the leading order term in \( \alpha' \) is proportional to \( \alpha_0^2 \alpha' \).