Statistical Physics IV: Non-equilibrium statistical physics
ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL)

Written exam

Part A (3pt/problem) - short questions

Please answer the following questions in brief and explain the concepts.

1. Write down Ito's lemma for a function $f(x)$ where $x(t)$ is a drift-diffusion stochastic process. Write down the definition of Wiener increment $dW(t)$ in the drift-diffusion process and its Ito's calculus rules (average of dW and average of dW^2).

2. Write down the 1D Langevin equation for Brownian motion, assuming the drag force experienced by the particle is given by
$$F = -\gamma m v, \tag{1}$$
where v and m are the particle velocity and mass. Write down the Langevin force thermal spectrum at temperature T.

3. If $\{x_i\}_{i=1,..,N}$ is a set of random variables with the same average $\langle x_i \rangle = a$ and variance $\langle (x_i - \langle x_i \rangle)^2 \rangle = b^2$, and N is a large number, find the probability distribution $P(X)$ of the arithmetic mean $X = \frac{1}{N}\sum_{i=1}^{N} x_i$.

4. Provide an example of probability distributions to which the central limit theorem is not applicable. Write down the probability density function for this distribution.

5. Derive Jarzynski equality from the Crooks theorem. Crooks theorem can be expressed in the following form:
$$\frac{P_F(W)}{P_B(-W)} = \exp\left(\frac{W - \Delta F}{k_B T}\right), \tag{2}$$
where $P_F(W)$ is the probability to perform work W over forward process, $P_B(W)$ is the probability to perform work W for backward process, ΔF is the free energy change between the initial and final states, T is the temperature and k_B is Boltzmann constant.

6. Find correlation functions $\langle \hat{a}^\dagger(t)\hat{a}(t+\tau)\rangle$ and $\langle \hat{a}(t)\hat{a}^\dagger(t+\tau)\rangle$ of an oscillator with frequency ω_0 and damping rate γ coupled to a bath at temperature T using quantum regression theorem,
$$\frac{d}{dt}\langle \hat{A}_\mu(t)\rangle = \sum_\nu M_{\mu\nu}\langle \hat{A}_\nu(t)\rangle, \tag{3}$$
$$\frac{d}{d\tau}\langle \hat{O}(t)\hat{A}_\mu(t+\tau)\rangle = \sum_\nu M_{\mu\nu}\langle \hat{O}(t)\hat{A}_\nu(t+\tau)\rangle. \tag{4}$$
Here $\hat{a}$ is the annihilation operator of the oscillator mode, and the mode occupation is given as $\langle \hat{n}(t)\rangle$.

7. Show that the classical spectral density of a (stable) stochastic process $S_{xx}[\omega] = \int_{-\infty}^{\infty}\langle x(t+\tau)x(t)\rangle e^{i\omega\tau}d\tau$ is always symmetric with respect to frequency ($S_{xx}[\omega] = S_{xx}[-\omega]$). Why its quantum counterpart $S_{xx}[\omega] = \int_{-\infty}^{\infty}\langle \hat{x}(t+\tau)\hat{x}(t)\rangle e^{i\omega\tau}d\tau$ may not be symmetric?

8. Write down the quantum master equation in the Lindblad form. What is the Lindblad operator for the dephasing of a harmonic oscillator?

Part B (6pt/problem)

Please pick 4 questions out of the following 5 and solve the corresponding exercises. Please indicate your choices on the first sheet.

1. The process X, defined by the Itô equation $dX = cX\,dW$, is known as a multiplicative white noise process, or geometric Brownian motion (GBM).

   (a) Define the process $Y = \log X$, and by using Itô's lemma, obtain its equation of motion

   (b) Integrate this equation, calculate $\langle X(t)\rangle$ and show that the covariance satisfies,

   $$\langle X(t)X(s)\rangle = \langle X(0)^2\rangle \exp\left(c^2 \min(t,s)\right).$$

   Hint: Use the formula $\langle \exp z\rangle = \exp\left(\frac{1}{2}\langle z^2\rangle\right)$, valid for any Gaussian random variable z with zero mean.

2. Consider an ensemble of atoms with two states E_1 and E_2, resonant with a mode of the radiation field of frequency $\omega = |E_2 - E_1|/\hbar$. The numbers of atoms in the ground and excited state are N_1 and N_2. According to the quantum theory of light the energy of the radiation field is quantized and obeys $E = n\hbar\omega$, where n is the number of photons in the radiation field. Transition from the ground state to the excited state absorbs a photon, and happens at a rate $r_n = n\gamma N_1$. Transition from the excited to the ground state creates a photon, and happens at a rate $g_n = (n+1)\gamma N_2$. The extra factor of one originates from *spontaneous emission*. We assume the numbers of atoms in each state N_1 and N_2 to be fixed by some other process and stay constant, so that we only consider the fluctuations of the photon number n.

   (a) Derive the master equation and solve it in the steady state.

   (b) Assume that $k_B T \gg |E_2 - E_1| = \hbar\omega$. If the atoms are in thermal equilibrium, it follows from the Boltzmann statistics that $N_2/N_1 = e^{-\hbar\omega/k_B T}$. Derive an expression for the steady state distribution of $P(n)$ and calculate $\langle n\rangle$. Show that this yields the Bose-Einstein statistics.

3. The generalized Langevin equation for a particle under damping is given as

   $$\dot{v} = -\int_0^t \gamma(t-t')v(t')dt' + \frac{F(t)}{m}. \tag{5}$$

   The generic solution of this equation of motion is

   $$v(t) = v(0)\cdot m\chi(t) + \int_0^t \chi(t-t')F(t')dt', \tag{6}$$

   where $\chi(t)$ is the inverse Fourier-Laplace transform of

   $$\chi(\omega) = v(\omega)/F(\omega) = \int_0^\infty e^{-i\omega t}\chi(t)dt. \tag{7}$$

   (a) Using the solution above, derive the generalized fluctuation dissipation theorem, i.e. find the spectrum of the random thermal force F defined as

   $$\int_{-\infty}^{+\infty} \langle F_{\text{th}}(t)F_{\text{th}}(0)\rangle e^{-i\omega t}dt. \tag{8}$$

   (b) The equation of motion for the current in a RLC series circuit is given by

   $$RI(t) + L\frac{dI(t)}{dt} + \frac{1}{C}\int_0^t I(t')dt' = V_{th}(t), \tag{9}$$

   where $V_{th}(t)$ is a thermally induced fluctuating voltage. Write down the spectrum of I and V_{th} using generalized fluctuation dissipation theorem.

4. Consider a harmonic oscillator coupled to a heat bath, consisting of a large ensemble of harmonic oscillators. The Hamiltonian of the system and the bath can be expressed as

$$\hat{H}_{\text{sys}} = \hbar\omega_s \left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \tag{10}$$

$$\hat{H}_{\text{bath}} = \sum_k \hbar\omega_k \left(\hat{b_k}^\dagger\hat{b}_k + \frac{1}{2}\right) \tag{11}$$

Here, $\hat{a}$ and $(\hat{a}^\dagger)$ are the annihilation and creation operators which satisfy the commutator relation $[\hat{a}, \hat{a}^\dagger] = 1$ and can be related to the position operator via $\hat{x}_{\text{sys}} = \sqrt{\frac{\hbar}{2m\Omega_m}}(\hat{a}^\dagger + \hat{a})$. Assume that the bath and the system are interacting in a bilinear way, i.e.that the interaction Hamiltonian takes the form:

$$\hat{H}_{int} = \hbar\sum_k g_k(\hat{a}\hat{b}_k^\dagger + \hat{b}_k\hat{a}^\dagger). \tag{12}$$

We also assume that the heat bath is in thermal equilibrium and has a finite temperature. This implies that $\langle\hat{b}_k^\dagger(0)\rangle = \langle\hat{b}_k(0)\rangle = 0$, as well as $\langle\hat{b}_k^\dagger(0)\hat{b}_l(0)\rangle = \delta_{k,l}\bar{n}_k$ and $\langle\hat{b}_k(0)\hat{b}_l^\dagger(0)\rangle = \delta_{k,l}(\bar{n}_k + 1)$, where $\bar{n}_k$ is the effective occupation number of the k^{th} mode. Finally, we assume that the bath modes are initially uncorrelated with each other, i.e. $\langle\hat{b_k}(0)\hat{b}_l^\dagger(0)\rangle = 0$ for $k \neq l$.

(a) Derive the Heisenberg equations of motion for the bath and system operators separately.

(b) Next, eliminate the bath operators from the equation of motion for $\hat{a}(t)$ by inserting the equation of the bath. Moreover, introduce the *density of states* $D(\omega)$ (that is, the number of modes in a given volume between ω and $\omega + \mathrm{d}\omega$) of the bath modes and convert the summation over k to an integral over ω, assuming that the coupling is frequency independent, i.e. $g_k = g(\omega_k) = g$ (this is called the 1st Markov approximation). Carry out the integration over ω using $\int_{-\infty}^{\infty} d\omega e^{-i\omega(t-t')} = 2\pi\delta(t - t')$.[1]

(c) Transform the equations of motion to a frame rotating with ω_s with respect to the original Hamiltonian $H_0 = H_{\text{sys}} + H_{\text{bath}}$. Show that the equation of motion for the system operator obeys the **Quantum Langevin Equation**:

$$\boxed{\frac{d}{dt}\hat{a}(t) = -\frac{\kappa}{2}\hat{a}(t) + \hat{F}(t)}$$

Give an expression for the Langevin noise term $\hat{F}(t)$ in terms of the bath operators.

5. Consider a simple quantum harmonic oscillator with mass m and frequency Ω. The oscillator is at a temperature T; this temperature is maintained through an infinitesimal coupling to a heat bath (therefore, one can neglect the energy decay rate κ of the oscillator). Let $\hat{x}$ and $\hat{p}$ denote the position and momentum operators (obeying the canonical commutation relation) and $\hat{a}$, $\hat{a}^\dagger$ the standard annihilation and creation operators.

(a) Show that the autocorrelation function of the position operator is given by

$$C_{xx}(t) \equiv \langle\hat{x}(t)\hat{x}(0)\rangle = \langle\hat{x}(0)\hat{x}(0)\rangle\cos(\Omega t) + \langle\hat{p}(0)\hat{x}(0)\rangle\frac{1}{M\Omega}\sin(\Omega t)$$

(b) Show that in thermal equilibrium the following expressions hold: $\langle\hat{x}(0)\hat{p}(0)\rangle = i\hbar/2$ and $\langle\hat{p}(0)\hat{x}(0)\rangle = -i\hbar/2$

[1] Note that this property also gives rise to the equality $\int_{t_0}^{t} c(t')\delta(t - t')dt' = \frac{1}{2}c(t)$, which is needed to derive the exact form of the quantum Langevin equation.

(c) Using these expressions, show that the autocorrelation function is given by

$$C_{xx}(t) \propto \bar{n}(\hbar\Omega)e^{i\Omega t} + [\bar{n}(\hbar\Omega) + 1]e^{-i\Omega t},$$

where $\bar{n}$ is the Bose-Einstein occupation factor. Calculate the proportionality factor.

(d) Using the correlation function above, calculate the spectral density $S_{xx}(\omega)$ and show that it is asymmetric in frequency. Show that in the high temperature limit ($k_B T \gg \hbar\Omega$), this spectral density becomes symmetric (thus, it coincides with the classical case).