Ex8492: Stochastic picture of sweep in 2-site system

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The problem:

Consider N classical particles in a two site system. The two sites are subjected to a potential difference ε. The temperature of the system is T. Define $n \in [-N, N]$ as the occupation difference. Assume that the thermalization process can be described by a stochastic rate equation

$$\frac{dn}{dt} = -\gamma n + A(t)$$

where $A(t)$ is a noisy term that reflects the fluctuations of the potential difference. Assuming that it has an average value A_ϵ and a power spectrum $\phi(\omega)$, it follows that n relaxes to an average value $\langle n \rangle_\epsilon$, with fluctuations that are characterized by a power spectrum $C(\omega)$ and intensity $\nu \equiv \tilde{C}(0)$.

(1) Write what is the interaction energy H_{int} of n with the field ε. Later you will have to be careful with the identification of the conjugate variables.

(2) Using the canonical formalism, find what are $\langle n \rangle_\epsilon$ and $\text{Var}(n)$. Additionally provide approximations for small ε.

(3) Determine what is A_ϵ such that $\langle n \rangle_\epsilon$ would be consistent with the canonical result. Assuming small ε deduce that $A_\epsilon \propto \epsilon$, and find the pre-factor.

(4) What is the $\chi(\omega)$ that characterizes the response of n to the applied potential in the linear-response regime? Assume that the dynamics are described by the stochastic rate equation; care to identify correctly the conjugate variables; and take into account your answer to item (3).

(5) Consider a quasi-static sweep process, namely, a process during which ϵ is varied slowly with constant rate $\dot{\epsilon}$. Use your result for $\chi(\omega)$ in order to express $\langle n \rangle$ in terms of $\langle n \rangle_\epsilon$ and $\dot{\epsilon}$.

(6) Deduce from the fluctuation-dissipation relation what is the correlation function $C(\tau)$ that describes the fluctuations. Explain how your answer in item (5) is related to the fluctuation intensity ν.

Advice: Care about factors of "2" in your answers. Failure to provide strictly correct pre-factors will be regarded as an essential error. Exploit item (6) in order to double check your answer in (5).

The solution:

(1) Let us consider a two site system, with N particles. The potential difference ε can be given by the following formulation: a particle in the first site has $-\varepsilon/2$ energy, while a particle in the second site has $\varepsilon/2$. The interaction Hamiltonian is described by

$$\mathcal{H}_{\text{int}} = -\frac{\varepsilon}{2}N_1 + \frac{\varepsilon}{2}N_2 = -\frac{\varepsilon}{2}n \tag{1}$$

Where N_1, N_2 are the occupation of the sites, and $n = N_1 - N_2$ is the occupation difference. Let us identify our conjugated variables

$$-\frac{\partial \mathcal{H}_{\text{int}}}{\partial n} = \frac{\varepsilon}{2} \tag{2}$$

(2) Let us calculate the partition function for a single particle

$$Z_1 = e^{-\frac{\beta\varepsilon}{2}} + e^{\frac{\beta\varepsilon}{2}} = 2\cosh\frac{\beta\varepsilon}{2} \tag{3}$$

The particles don't interact with each other, therefore the sum over states can be factorized and we have

$$Z = \left(2\cosh\frac{\beta\varepsilon}{2}\right)^N \tag{4}$$

This is the partition function for N particles. We calculate $\langle n \rangle$ in the following manner

$$\langle n \rangle = -\frac{2}{\varepsilon}\langle \mathcal{H}_{\text{int}} \rangle = -\frac{2}{\varepsilon}E = \frac{2}{\varepsilon}\frac{\partial}{\partial\beta}\ln Z = N\frac{\sinh\frac{\beta\varepsilon}{2}}{\cosh\frac{\beta\varepsilon}{2}} = N\tanh\frac{\beta\varepsilon}{2} \tag{5}$$

We notice that in the limit $\varepsilon \to 0$ we have $\langle n \rangle \to 0$ and in the limit $\varepsilon \to \infty$ we have $\langle n \rangle \to N$, as expected. Using the same logic as before we substitute into the known variance equation

$$\text{Var}\,(n) = \frac{4}{\varepsilon^2}\text{Var}\,(E) = \frac{4}{\varepsilon^2}\frac{\partial^2}{\partial\beta^2}\ln Z = \frac{4}{\varepsilon^2}\frac{\partial}{\partial\beta}\left(N\frac{\varepsilon}{2}\tanh\frac{\beta\varepsilon}{2}\right) = \frac{N}{\cosh^2\frac{\beta\varepsilon}{2}} \tag{6}$$

For the approximation of small ε we have

$$\langle n \rangle \approx \frac{N\beta}{2}\varepsilon \tag{7}$$

And for the variance we obtain

$$\text{Var}\,(n) \approx N \tag{8}$$

(3) We take the average of the rate equation in steady state, and compare it with the canonical result to find the pre-factor

$$\left\langle \frac{\mathrm{d}n}{\mathrm{d}t} \right\rangle = -\gamma\,\langle n \rangle + \langle A\,(t) \rangle = 0 \Rightarrow A_0 = \gamma\,\langle n \rangle \tag{9}$$

Hence in the small ε approximation using Eq. (7) we have

$$A_\epsilon = \frac{N\beta\gamma}{2}\varepsilon \tag{10}$$

(4) By Using the Fourier transform on our rate equation, and substituting the result from the previous paragraph we have

$$-i\omega n_\omega = -\gamma n_\omega + N\beta\gamma\frac{\varepsilon_\omega}{2} \Rightarrow n_\omega = N\beta\gamma\frac{1}{-i\omega+\gamma}\frac{\varepsilon_\omega}{2} \tag{11}$$

From which we derive an expression for $\chi(\omega)$, one should be careful and remember the correct conjugate variables which we found in Eq. (2)

$$\chi\,(\omega) = N\beta\gamma\frac{1}{\gamma - i\omega} = N\beta\gamma\frac{i\omega+\gamma}{\gamma^2+\omega^2} \tag{12}$$

(5) Using Kubo formula for the dissipation coefficient (AC version)

$$\eta(\omega) \equiv \frac{Im[\chi(\omega)]}{\omega} = \frac{\gamma N\beta}{\gamma^2+\omega^2} \tag{13}$$

Hence, for the D.C limit we get

$$\eta_{D.C} = \frac{N\beta}{\gamma} \tag{14}$$

So according the linear response theory

$$\langle n \rangle = \langle n \rangle_\epsilon - \frac{N\beta}{\gamma}\frac{\dot{\epsilon}}{2} \tag{15}$$

(6) Using the fluctuation dissipation relation (FDR) AC version, under the canonical preparation assumption

$$\mathrm{Im}\left[\chi\left(\omega\right)\right] = \tanh\left(\frac{\omega}{2T}\right) C\left(\omega\right) \tag{16}$$

In the classical limit, which is obtained by taking the small ω limit, we have $\tanh\left(\omega/2T\right) \approx \omega/2T$. Solving for the power spectrum we obtain

$$C\left(\omega\right) = \frac{2T}{\omega} N\beta\gamma \frac{\omega}{\gamma^2+\omega^2} = 2N\gamma\frac{1}{\gamma^2+\omega^2} \tag{17}$$

For consistency let us remember that the relation of the power spectrum to the variance is the inverse Fourier transform at $\tau = 0$. From the well known Fourier transform of a Lorenzian we obtain

$$C\left(\tau\right) = \mathrm{F.T.}^{-1}\left[C\left(\omega\right)\right] = Ne^{-\gamma|\tau|} \tag{18}$$

And as expected we get

$$\nu \equiv C\left(\omega = 0\right) = \frac{2N}{\gamma} \tag{19}$$

$$\eta = \frac{\nu\beta}{2} \tag{20}$$