Ex8490: Stochastic rate equation

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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. In items (3-6) 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_0 and a power spectrum $\phi(\omega)$, it follows that n relaxes to an average value $\langle n \rangle$, with fluctuations that are characterized by a power spectrum $C(\omega)$.

(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 $\langle n \rangle$ and $\text{Var}(n)$. Additionally provide approximations for small ε.

(3) Determine what is A_0 such that $\langle n \rangle$ would be consistent with the canonical result. Assuming small ε deduce that $A_0 \propto \epsilon$, 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) Deduce from the fluctuation-dissipation relation what is the power spectrum $C(\omega)$. Care to use the appropriate definition for $\chi(\omega)$, else the result will come out wrong.

(6) Deduce what is the power spectrum $\phi(\omega)$ that is required in order to reproduce $C(\omega)$ from the stochastic rate equation.

Advice: In item (5) verify that your result is consistent with the answer to item (2). Likewise you can debug the numerical pre-factor in your answer to item (6). Care about factors of "2" in your answers. Failure to provide strictly correct pre-factors will be regarded as an essential error.

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

$$A_0 = \frac{N\beta\gamma}{2}\varepsilon \tag{10}$$

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

$$\text{Im}\left[\chi\,(\omega)\right] = \tanh\left(\frac{\omega}{2T}\right)C\,(\omega) \tag{13}$$

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

$$C\left(\omega\right) = \frac{2T}{\omega} N\beta\gamma \frac{\omega}{\gamma^2 + \omega^2} = 2N\gamma \frac{1}{\gamma^2 + \omega^2} \tag{14}$$

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

$$\text{F.T.}^{-1}\left[C\left(\omega\right)\right] = Ne^{-\gamma|\tau|} \tag{15}$$

This yields $C\left(\tau = 0\right) = N$ which is consistent with our previous results.

(6) We solve this *via* the rate equation in Fourier-space which leads to

$$\mathcal{C}\left(\omega\right) = \left(\omega^2 + \gamma^2\right)^{-1} \phi\left(\omega\right) \tag{16}$$

Solving for ϕ we have

$$\phi\left(\omega\right) = \left(\omega^2 + \gamma^2\right) C\left(\omega\right) = 2N\gamma \tag{17}$$