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) Determined 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 is 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:

Wrong factor of 2 throughout, and last item cumbersome

1. Let us consider a two site system, with N particles hopping between them. Assume that the potential difference ε is given by the fact that a particle in the first site receives $-\varepsilon/2$ to its energy, while a particle on the second site receives $\varepsilon/2$. The interaction is described by the following interaction Hamiltonian:

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

Here N_1, N_2 are the occupation of the first and second sites and $n = N_1 - N_2 = 2N_1 - N$ is the occupation difference.

2. There are a few different ways to find $\langle n \rangle$. Let us calculate the partition function for 1 particle:

$$Z_1 = 2\cosh\frac{\beta\varepsilon}{2}\,. \tag{2}$$

The indistinguishable particles don't interact with each other, so we have

$$Z = \frac{1}{N!}\left(2\cosh\frac{\beta\varepsilon}{2}\right)^N\,, \tag{3}$$

which is the partition function for N particles. The simplest way of calculating $\langle n \rangle$ is by noticing that $\langle n \rangle = 2\frac{\langle E \rangle}{-\varepsilon}$, so

$$\langle n \rangle = \frac{2}{\varepsilon}\frac{\partial \ln Z}{\partial \beta} = N\frac{\sinh\frac{\beta\varepsilon}{2}}{\cosh\frac{\beta\varepsilon}{2}} = N\tanh\frac{\beta\varepsilon}{2}\,. \tag{4}$$

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.
In the same way we say that $\mathrm{Var}\,(n) = 4\mathrm{Var}\,(E)\,/\varepsilon^2$, so

$$\mathrm{Var}\,(n) = \frac{4}{\varepsilon^2}\mathrm{Var}\,(E) = -\frac{4}{\varepsilon^2}\frac{\partial E}{\partial \beta} = -\frac{4}{\varepsilon^2}\frac{\partial}{\partial \beta}\left(-N\frac{\varepsilon}{2}\tanh\frac{\beta\varepsilon}{2}\right) = \frac{N}{\cosh^2\frac{\beta\varepsilon}{2}}\,. \tag{5}$$

In the limit of small ε we have:

$$\langle n \rangle \approx \frac{N\beta}{2}\varepsilon\,, \tag{6}$$

and (first non-zero term in the expansion)

$$\mathrm{Var}\,(n) \approx N\,. \tag{7}$$

3. Taking the average of the rate equation in accordace with the canonical result (steady state), we have

$$\left\langle \frac{\mathrm{d}n}{\mathrm{d}t} \right\rangle = -\gamma\langle n \rangle + \langle A\,(t) \rangle \Rightarrow A_0 = \gamma\langle n \rangle\,, \tag{8}$$

so in the small ε approximation we have:

$$A_0 = \frac{N\gamma\beta}{2}\varepsilon\,. \tag{9}$$

4. By inspecting the rate equation and taking the Fourier transform we get:

$$-i\omega n_\omega = -\gamma n_\omega + \frac{N\beta\gamma}{2}\varepsilon_\omega\,, \tag{10}$$

which immediately implies that $\chi\,(\omega)$ is:

$$\chi\,(\omega) = \frac{N\gamma\beta}{2}\frac{1}{\gamma - i\omega} = \frac{N\gamma\beta}{2}\frac{\gamma + i\omega}{\gamma^2 + \omega^2}\,. \tag{11}$$

5. The fluctuation dissipation relation reads:

$$\mathrm{Im}\left[\chi\left(\omega\right)\right]=\tanh\left(\frac{\omega}{2T}\right)C\left(\omega\right)\,, \tag{12}$$

in the DC limit we have $\tanh\left(\omega/2T\right)\approx\omega/2T$ and the power spectrum is:

$$C\left(\omega\right)=\frac{2T}{\omega}\frac{N\gamma\beta}{2}\frac{\omega}{\gamma^{2}+\omega^{2}}=\frac{N}{\gamma}\frac{1}{1+\left(\omega/\gamma\right)^{2}}\,. \tag{13}$$

A nice way to check this result is to see whether $C\left(\tau=0\right)$ coincides with $\mathrm{Var}\left(n\right)\approx N$, in order to do so we calculate $\mathrm{F.T.}^{-1}\left[C\left(\omega\right)\right]$:

$$\mathrm{F.T.}^{-1}\left[C\left(\omega\right)\right]=Ne^{-\tau\gamma}\,, \tag{14}$$

which gives $C\left(\tau=0\right)=N$ as it should!

6. Let us multiply the rate equation for time t' by the same equation for time t''. The result is as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t'}\frac{\mathrm{d}}{\mathrm{d}t''}n\left(t'\right)n\left(t''\right)+\gamma n\left(t'\right)\frac{\mathrm{d}}{\mathrm{d}t''}n\left(t''\right)+\gamma n\left(t''\right)\frac{\mathrm{d}}{\mathrm{d}t'}n\left(t'\right)+\gamma^{2}n\left(t'\right)n\left(t''\right)= \tag{15}$$

$$=A\left(t'\right)A\left(t''\right)\,. \tag{16}$$

Taking the average of the above equation, and going to a new variable $\tau=t'-t''$ we have:

$$-\frac{\mathrm{d}^{2}}{\mathrm{d}\tau^{2}}C\left(\tau\right)+\gamma^{2}C\left(\tau\right)=\phi\left(\tau\right)\,. \tag{17}$$

Taking the Fourier transform we get:

$$\left(\omega^{2}+\gamma^{2}\right)C\left(\omega\right)=\phi\left(\omega\right)\,. \tag{18}$$

This gives $\phi\left(\omega\right)=N\gamma$, meaning that $\phi\left(\tau\right)=N\gamma\delta\left(\tau\right)$, both of them have the appropriate dimensions.