Ex7010: Site occupation during a sweep process

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The problem:
Consider the occupation n of a site whose binding energy ε can be controlled, say by changing a gate voltage. The temperature of the environment is T and its chemical potential is μ. Consider separately 3 cases:

(a) The occupation n can be either 0 or 1.
(b) The occupation n can be any natural number $(0, 1, 2, 3, ...)$
(c) The occupation n can be any real positive number $\in [0, \infty]$

We define $\bar{n}$ as the average occupation at equilibrium. The fluctuations of $\delta n(t) = n(t) - \bar{n}$ are characterized by a correlation function $C(\tau)$. Assume that it has exponential relaxation with time constant τ_0. Later we define $\langle n \rangle$ as the average occupation during a sweep process, where the potential is varied with rate $\dot{\varepsilon}$.

(1) Calculate $\bar{n}$, express it using (T, ε, μ).

(2) Calculate $\text{Var}(n)$, express the result using $\bar{n}$.

(3) Write an expression for the $\omega = 0$ intensity ν of the fluctuations.

(4) Write an expression for $\langle n \rangle$ during a sweep process.

The solution: Irrespective of whether you have solved (1) and (2), in item (3) express the result using $\text{Var}(n)$. In item (4) use the classical version of the fluctuation-dissipation relation, and express the result using $(T, \tau_0, \bar{n}, \dot{\varepsilon})$, where $\bar{n}$ had been given by your answer to item (1). Note that the time dependence is *implicit* via $\bar{n}$.

1 Average occupation at equilibrium

The energy for n patrticles is $E_n = n\epsilon$. The probability for n particles is:

$$p_n = \frac{1}{Z} e^{-\beta(\epsilon-\mu)n}$$

(a) There are only two options $n = 0, 1$; then $Z = 1 + e^{-\beta(\epsilon-\mu)}$. And the average occupation:

$$\bar{n} = \sum_0^1 p_n n = \frac{e^{-\beta(\epsilon-\mu)}}{1 + e^{-\beta(\epsilon-\mu)}} = \frac{1}{e^{\beta(\epsilon-\mu)} + 1} \tag{1}$$

(b) Similarly to the previous case, but $n = 0, 1, 2....$ The partition function:

$$Z = \sum_{n=0}^{\infty} e^{-\beta(\epsilon-\mu)n} = \frac{1}{1 - e^{-\beta(\epsilon-\mu)}} \tag{2}$$

And the average occupation:

$$\bar{n} = \sum_{n=0}^{\infty} p_n n = \frac{1}{Z} \sum_{n=0}^{\infty} n e^{-\beta(\epsilon-\mu)n} \tag{3}$$

$$= \frac{1}{Z\beta}\frac{\partial}{\partial\mu}\sum_{n=0}^{\infty} e^{-\beta(\epsilon-\mu)n} = \frac{1}{Z\beta}\frac{\partial Z}{\partial\mu} = e^{-\beta(\epsilon-\mu)}\frac{e^{-\beta(\epsilon-\mu)}}{(1-e^{-\beta(\epsilon-\mu)})^2} = \frac{1}{e^{\beta(\epsilon-\mu)}-1}$$

(c) The partition function:

$$Z = \int_0^{\infty} e^{-\beta(\epsilon-\mu)n}dn = \frac{1}{\beta(\epsilon-\mu)} \tag{4}$$

And the average occupation:

$$\bar{n} = \int_0^{\infty} np_n dn = \frac{1}{Z}\int_0^{\infty} ne^{-\beta(\epsilon-\mu)n}dn = \frac{1}{Z\beta}\frac{\partial}{\partial\mu}\int_0^{\infty} e^{-\beta(\epsilon-\mu)n}dn = \frac{1}{Z\beta}\frac{\partial Z}{\partial\mu} \tag{5}$$

$$= \frac{\beta(\epsilon-\mu)}{(\beta(\epsilon-\mu))^2} = \frac{1}{\beta(\epsilon-\mu)}$$

2 Variance of the occupation

(a) In this case $\langle n^2\rangle = \langle n\rangle$ (see eq(1)):

$$\langle n^2\rangle = \sum_{n=0}^{1} n^2 p_n = p_1 = \sum_{0}^{1} p_n n = \bar{n} \tag{6}$$

The variance is:

$$\mathrm{Var}(n) = \langle n^2\rangle - \langle n\rangle^2 = \bar{n} - \bar{n}^2 = \bar{n}(1-\bar{n}) \tag{7}$$

(b) The average of n^2:

$$\langle n^2\rangle = \sum_{n=0}^{\infty} p_n n^2 = -\frac{1}{Z\beta^2}\frac{\partial^2 Z}{\partial\mu^2} \tag{8}$$

And the variance is:

$$\mathrm{Var}(n) = \langle n^2\rangle - \langle n\rangle^2 = \frac{1}{\beta^2}\frac{\partial}{\partial\mu}(\frac{1}{Z}\frac{\partial Z}{\partial\mu}) = \frac{\partial\langle n\rangle}{\partial\beta\mu}$$

$$= -\frac{1}{(e^{\beta(\epsilon-\mu)+1})^2}(-e^{\beta(\epsilon-\mu)}) = \frac{1}{(e^{\beta(\epsilon-\mu)+1})^2}(e^{\beta(\epsilon-\mu)} - 1 + 1) = \bar{n}(1+\bar{n}) \tag{9}$$

(c) In this case:

$$\langle n^2\rangle = \int_0^{\infty} p_n n^2 dn = \frac{1}{Z\beta^2}\frac{\partial^2 Z}{\partial\mu^2} \tag{10}$$

And the variance is:

$$\mathrm{Var}(n) = \frac{1}{\beta^2}\frac{\partial}{\partial\mu}(\frac{\partial \ln Z}{\partial\mu}) = \frac{1}{\beta}\frac{\partial}{\partial\mu}(\frac{1}{\beta(\epsilon-\mu)}) = \frac{1}{\beta^2(\epsilon-\mu)^2} = \bar{n}^2 \tag{11}$$

3 Intensity of the fluctuations

The fluctuations of $\delta n(t) = n(t) - \bar{n}$ are characterized by a correlation function $C(\tau)$ assuming that it has exponential relaxation with time constant τ_0. Hence:

$$C(\tau) = \langle \delta n(t) \delta n(0) \rangle = \mathrm{Var}(n) \exp(-\frac{|\tau|}{\tau_0}) \tag{12}$$

Where the pre-factor $\mathrm{Var}(n)$ comes from the $C(\tau = 0)$ result.
The intensity ν is :

$$\nu = \tilde{C}(\omega = 0) = \mathrm{Var}(n) \int_{-\infty}^{+\infty} \exp(-\frac{|\tau|}{\tau_0}) d\tau = 2\,\mathrm{Var}(n) \int_0^{+\infty} e^{-\frac{\tau}{\tau_0}} d\tau = 2\,\mathrm{Var}(n)\tau_0 \tag{13}$$

4 $\langle n \rangle$ during a sweep process

The conjucaeted variable to n is $-\epsilon$:

$$-\frac{\partial \mathcal{H}}{\partial n} = -\epsilon \tag{14}$$

From linear response we have:

$$\langle F \rangle_t = \langle F \rangle_X - \eta \dot{X} \tag{15}$$

where in our case the output signal $\langle F \rangle_t$ here is $\langle n \rangle_t$, and the input signal X is $-\epsilon$.
The intensity of the fluctuations:

$$\eta = \frac{\nu}{2T} = \frac{\tau_0}{T} \mathrm{Var}(n) \tag{16}$$

$\langle n \rangle_t$ during a sweep process:

$$\langle n \rangle_t = \bar{n} + \dot{\epsilon}\eta = \bar{n} + \frac{\dot{\epsilon}\tau_0}{T} \mathrm{Var}(n) \tag{17}$$