Statistical Mechanics - Class Exercise 10

January 10, 2023

Exercise 7010 - Site occupation during a sweep process

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 $\dot{\epsilon}$.

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.

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 $(T, \tau_0, \bar{n}, \dot{\epsilon})$, where $\bar{n}$ had been given by your answer to item (1). Note that the time dependence is implicit via $\bar{n}$.

Answer

1. The energy for n particles is $E_n = n\epsilon$.
The probability for n particles is $p_n = \frac{1}{Z} e^{-\beta(\epsilon-\mu)n}$
the average occupation

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

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

$$\bar{n} = \frac{1}{\beta} \frac{\partial \ln(Z)}{\partial \mu} = \frac{e^{-\beta(\epsilon-\mu)}}{1 + e^{-\beta(\epsilon-\mu)}} = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}$$

we get a Fermi-Dirac occupation.

(b) Now $n = 0, 1, 2....$ The partition function:

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

And the average occupation:

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

we get a Bose–Einstein occupation.
(c) The partition function:

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

And the average occupation:

$$\bar{n} = \frac{1}{\beta}\frac{\partial \ln(Z)}{\partial \mu} = \frac{1}{\beta(\epsilon-\mu)}$$

The last case is like the high temperature approximation of the previous case
2. The variance is:

$$\mathrm{Var}(n) = \langle n^2 \rangle - \langle n \rangle^2$$

$$\langle n^2 \rangle = \sum p_n n^2 = \frac{1}{Z}\sum n^2 e^{-\beta(\epsilon-\mu)n} = \frac{1}{Z\beta^2}\frac{\partial^2 Z}{\partial \mu^2}$$

$$\langle n \rangle^2 = \bar{n}^2 = \frac{1}{Z^2\beta^2}\left(\frac{\partial Z}{\partial \mu}\right)^2$$

$$\mathrm{Var}(n) = \langle n^2 \rangle - \langle n \rangle^2 = \frac{1}{\beta^2}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial \mu^2} - \frac{1}{Z^2}\left(\frac{\partial Z}{\partial \mu}\right)^2\right] = \frac{1}{\beta^2}\frac{\partial^2 \ln(Z)}{\partial \mu^2} = \frac{1}{\beta}\frac{\partial \bar{n}}{\partial \mu}$$

So we get
(a)

$$\mathrm{Var}(n) = \frac{1}{\beta}\frac{\partial \bar{n}}{\partial \mu} = \frac{e^{\beta(\epsilon-\mu)}}{\left(e^{\beta(\epsilon-\mu)} + 1\right)^2} = \frac{e^{\beta(\epsilon-\mu)} + 1 - 1}{\left(e^{\beta(\epsilon-\mu)} + 1\right)^2} = \bar{n}\left(1 - \bar{n}\right)$$

(b)

$$\mathrm{Var}(n) = \frac{1}{\beta}\frac{\partial \bar{n}}{\partial \mu} = \frac{e^{\beta(\epsilon-\mu)}}{\left(e^{\beta(\epsilon-\mu)} - 1\right)^2} = \frac{e^{\beta(\epsilon-\mu)} - 1 + 1}{\left(e^{\beta(\epsilon-\mu)} - 1\right)^2} = \bar{n}\left(1 + \bar{n}\right)$$

(c)

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

3. 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:

$$C(\tau) = \langle \delta n(\tau)\delta n(0) \rangle = Ae^{-\frac{|\tau|}{\tau_0}}$$

For $C(0) = \langle (\delta n(0))^2 \rangle = \mathrm{Var}(n) = A$, so

$$C(\tau) = \mathrm{Var}(n)e^{-\frac{|\tau|}{\tau_0}}$$

The intensity

$$\nu = \tilde{C}\left(\omega = 0\right) = \int_{-\infty}^{\infty} C(\tau)d\tau = \text{Var}(n)\int_{-\infty}^{\infty} e^{-\frac{|\tau|}{\tau_0}}d\tau = 2\text{Var}(n)\int_{0}^{\infty} e^{-\frac{\tau}{\tau_0}}d\tau = 2\text{Var}(n)\tau_0$$

$$\rightarrow C(\tau) = \frac{\nu}{2\tau_0}e^{-\frac{|\tau|}{\tau_0}}$$

4. The conjugated variable to n is $-\epsilon$:

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

From linear response we have:

$$\langle F \rangle_t = \chi X$$

$$\langle F \rangle_\omega = \left(\text{Re}\chi_\omega + i\text{Im}\chi\right)X = \left(\chi_0 X + i\omega\eta X\right)$$

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

where in our case the output signal $\langle F \rangle_t$ here is $\langle n \rangle_t$, and the input signal X is $-\epsilon$.
η is the imaginary part of the generalized susceptibility and from FDT we get

$$\eta = \frac{\text{Im}\left[\chi\left(\omega\right)\right]}{\omega} = \frac{1}{\hbar\omega}\tanh\left(\frac{\hbar\omega}{2T}\right)\tilde{C}\left(\omega\right)$$

In the classical version $\omega \rightarrow 0$ and we get the intensity of the fluctuations:

$$\eta = \frac{\nu}{2T} = \frac{\tau_0}{T}\text{Var}(n)$$

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

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

Exercise 7040 - FDT for RL-circuit, Nyquist theory

Derive the Nyquist expression for the current-current correlation function in a closed ring, taking into account its inductance. Use the following procedure:

1. Cite an expression for the inductance L of a torus shaped ring given its radius R and its cross-section radius r.
2. Write the R-L circuit equation for the current I, where the flux $\Phi(t)$ through the ring is the driving parameter.
3. Identify the generalized susceptibility $\chi(\omega)$.
4. Calculate the current-current correlation function $\langle I(t)I(0)\rangle$, taking the classical / high temperature limit.
5. Verify that $\langle I^2 \rangle$ agree with the canonical result.

Answer

1.

$$L = \mu_0 R \left[ln \left(\frac{8R}{r} \right) - 1.75 \right]$$

(See https://en.wikipedia.org/wiki/Inductance)

2. For a closed ring with the flux $\Phi(t)$ through the ring, the electromotive force

$$\dot{\Phi} = RI - L\dot{I}$$

By taking Transform Fourier of the equation we get

$$i\omega\Phi_\omega = RI_\omega - i\omega L I_\omega$$

$$I_\omega = \frac{i\omega\Phi_\omega}{(R - i\omega L)}$$

3. From the last equation we get

$$I_\omega = \frac{i\omega}{(R - i\omega L)}\Phi_\omega$$

So, the generalized susceptibility

$$\chi(\omega) = \frac{i\omega}{(R - i\omega L)}$$

4. We get

$$\chi(\omega) = \frac{i\omega}{(R - i\omega L)} = -\frac{\omega^2 L}{(R^2 + \omega^2 L^2)} + i\frac{\omega R}{(R^2 + \omega^2 L^2)} = \mathrm{Re}\chi(\omega) + i\mathrm{Im}\chi(\omega)$$

from FDT we know that

$$\eta = \frac{\mathrm{Im}\left[\chi(\omega)\right]}{\omega} = \frac{1}{\hbar\omega} \tanh\left(\frac{\hbar\omega}{2T}\right) \tilde{C}^{II}(\omega)$$

taking the classical / high temperature limit we get

$$\frac{\mathrm{Im}\left[\chi(\omega)\right]}{\omega} = \frac{R}{(R^2 + \omega^2 L^2)} = \frac{1}{2T}\tilde{C}^{II}(\omega) \to \tilde{C}^{II}(\omega) = \frac{T}{L}\frac{2\left(\frac{R}{L}\right)}{\left(\left(\frac{R}{L}\right)^2 + \omega^2\right)}$$

The current-current correlation function in the classical limit $\langle I(t)I(0)\rangle = C^{II}(t)$ is the Transform Fourier of $\tilde{C}^{II}(\omega)$

$$C^{II}(t) = \int_{-\infty}^{\infty} \tilde{C}^{II}(\omega) e^{i\omega t} \frac{d\omega}{2\pi} = \frac{2TR}{L^2}\int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\left(\left(\frac{R}{L}\right)^2 + \omega^2\right)}\frac{d\omega}{2\pi} =$$

$$= \frac{2TR}{L^2}\int_{-\infty}^{\infty} \frac{e^{i\omega t}}{\left(\omega - i\frac{R}{L}\right)\left(\omega + i\frac{R}{L}\right)}\frac{d\omega}{2\pi} = \frac{2TR}{L^2}(2\pi i)\frac{e^{-\frac{R}{L}t}}{\left(i\frac{R}{L} + i\frac{R}{L}\right)}\frac{1}{2\pi} = \frac{T}{L}e^{-\frac{R}{L}t}$$

5. By taking $t \to 0$ we get

$$C^{II}(0) = \langle I(0)I(0)\rangle = \left\langle I^2 \right\rangle = \frac{T}{L}$$

The Hamiltonian is $\mathcal{H} = \frac{1}{2}LI^2$ by using equal division rule for each quadratic term in the Hamiltonian we get the same result

$$\left\langle \frac{1}{2}LI^2 \right\rangle = \frac{T}{2}$$

and therefore

$$\langle I^2 \rangle = \frac{T}{L}$$