

Exercise 3.1 Relaxation of Polarized Spins Coupled to a Bath

Consider a system S of $N^{(S)}$ units with two states (spins $\uparrow^{(S)}$ and $\downarrow^{(S)}$) that are coupled to a reservoir R (infinitely larger than S) consisting of other two-state units (labeled as $\uparrow^{(R)}$ and $\downarrow^{(R)}$). This is a simplified model for nuclear spins in a metal, whereby the nuclear spins represent our system and the electrons (electron spins) the reservoir.

We assume that the microstates in S and R are non-degenerate with an energy difference $\Delta\epsilon$,

$$E_{\uparrow}^{(S)} - E_{\downarrow}^{(S)} = E_{\uparrow}^{(R)} - E_{\downarrow}^{(R)} = \Delta\epsilon, \quad (1)$$

where $E_{\uparrow}^{(S)}$ and $E_{\downarrow}^{(S)}$ ($E_{\uparrow}^{(R)}$ and $E_{\downarrow}^{(R)}$) are the energies for the two states in S (R).

The reservoir R is in its thermodynamic equilibrium such that the occupation probabilities $w_{\uparrow}^{(R)}$ and $w_{\downarrow}^{(R)}$ of the two states satisfy the relation,

$$\frac{w_{\uparrow}^{(R)}}{w_{\downarrow}^{(R)}} = \exp \left\{ -\frac{\Delta\epsilon}{k_B T^{(R)}} \right\}, \quad (2)$$

where $T^{(R)}$ defines the temperature of R . At the initial time, $t = 0$, S shall not be in equilibrium with R .

There is a coupling between the units of S and R in the following way. A spin of S can only be reversed, if simultaneously a spin of R is flipped in the opposite way, i.e.: $\uparrow^{(S)} \rightarrow \downarrow^{(S)}$ together with $\downarrow^{(R)} \rightarrow \uparrow^{(R)}$ and $\downarrow^{(S)} \rightarrow \uparrow^{(S)}$ together with $\uparrow^{(R)} \rightarrow \downarrow^{(R)}$. This corresponds to spin conservation as well as energy conservation.

Both types of processes occur with the same probability Γ (time reversal invariance):

$$|\dots, \uparrow, \dots\rangle^{(S)} \otimes |\dots, \downarrow, \dots\rangle^{(R)} \xrightarrow{\Gamma} |\dots, \downarrow, \dots\rangle^{(S)} \otimes |\dots, \uparrow, \dots\rangle^{(R)} \quad (3)$$

$$|\dots, \downarrow, \dots\rangle^{(S)} \otimes |\dots, \uparrow, \dots\rangle^{(R)} \xrightarrow{\Gamma} |\dots, \uparrow, \dots\rangle^{(S)} \otimes |\dots, \downarrow, \dots\rangle^{(R)} \quad (4)$$

From this consideration the effective transition rates ($\Gamma_{\uparrow\downarrow}$, $\Gamma_{\downarrow\uparrow}$) for the spins in S depend on the probabilities of finding states $\uparrow^{(R)}$ and $\downarrow^{(R)}$ in R , such that

$$\Gamma_{\uparrow\downarrow}^{(S)} = \Gamma w_{\downarrow}^{(R)}, \quad \Gamma_{\downarrow\uparrow}^{(S)} = \Gamma w_{\uparrow}^{(R)}. \quad (5)$$

- Formulate the master equation for the system S where $N_{\uparrow}^{(S)}$ and $N_{\downarrow}^{(S)}$ denote the occupation numbers of the two spin states ($N_{\uparrow}^{(S)} + N_{\downarrow}^{(S)} = N^{(S)}$). What does the condition of detailed balance imply?
- Compute the time dependent polarization of the localized spin system, defined by $P^{(S)}(t) = (N_{\uparrow}^{(S)}(t) - N_{\downarrow}^{(S)}(t))/N^{(S)}$, for the following starting conditions at $t = 0$:
 - unpolarized case ($N_{\uparrow}^{(S)} = N_{\downarrow}^{(S)}$),
 - almost completely polarized in the \downarrow -direction ($N_{\downarrow}^{(S)} = N^{(S)}(1 - \delta)$, $N_{\uparrow}^{(S)} = N^{(S)}\delta$, $\delta \ll 1$),

- (iii) almost completely polarized in the \uparrow -direction ($N_{\uparrow}^{(S)} = N^{(S)}(1 - \delta)$, $N_{\downarrow}^{(S)} = N^{(S)}\delta$, $\delta \ll 1$)

Determine the relaxation time for these three cases. Find the temperature $T^{(S)}$ of the spin system as a function of time (the temperature for S is defined similar to the temperature of the reservoir, Eq. (2)). Consider the initial temperatures, how do you explain the sign of $T^{(S)}$?

- c) Calculate the H -function of S and its derivative with respect to time for the three cases in b). Moreover, calculate the energy exchange between S and R as a function of t (take the temperature of the reservoir $T^{(R)}$ as a parameter) for the same three cases. Calculate the specific heat of S as a function of temperature $T^{(S)}$.

Hint: Set the zero of energy at $w_{\downarrow}^{(S)}$. You now know the energy of $w_{\uparrow}^{(S)}$, and hence also the entire internal energy of S .

Exercise 3.2 The Linear Boltzmann Equation

We want to study the Boltzmann equation when only one-particle scattering is considered, contrary to two-particle scattering as presented in the lecture. Let us consider a system of particles embedded in a static background of impurities such that one particle with momentum \vec{p} has a certain probability to be scattered to a new state with momentum \vec{p}' (e.g. electrons with an external potential from which they may scatter). We assume that the scattering processes are instantaneous, elastic and isotropic.

- a) Following the approach of the lecture notes, derive the Boltzmann equation of the system.
- b) List the quantities which are conserved in the one-particle collision and verify the relation

$$\int d^3p \varphi(\vec{p}) \left(\frac{\partial f(\vec{r}, \vec{p}, t)}{\partial t} \right)_{\text{coll}} = 0, \quad (6)$$

where $\varphi(\vec{p})$ denotes a conserved quantity (we use the notations of the lecture notes).

- c) Prove the “ H -theorem” discussing the assumptions you make. Find the equilibrium state and give the physical interpretation of a relaxation process towards equilibrium (what does it change in the system?).

Office Hours: Monday, October 8, 8 – 10 am (Evert van Nieuwenburg, HIT K 12.3)