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 $\Delta \epsilon$,

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

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

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: $\uparrow^{(S)} \to \downarrow^{(S)}$ together with $\downarrow^{(R)} \to \uparrow^{(R)}$ and $\downarrow^{(S)} \to \uparrow^{(S)}$ together with $\uparrow^{(R)} \to \downarrow^{(R)}$. This corresponds to spin conservation as well as energy conservation.

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

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

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

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

- a) 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?
- b) 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:
 - (i) unpolarized case $(N_{\uparrow}^{(S)} = N_{\downarrow}^{(S)}),$
 - (ii) almost complete polarized in \downarrow -direction $(N_{\downarrow}^{(S)} = N^{(S)}(1 \delta), N_{\uparrow}^{(S)} = N^{(S)}\delta, \delta \ll 1),$

(iii) almost complete polarized in \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 of the spin system $T^{(S)}$ for the three initial conditions (the temperature for S is defined similar to the temperature of the reservoir, Eq. (2)). 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. How does the temperature $T^{(S)}$ evolve as a function of time? Calculate the specific heat of S as a function of temperature $T^{(S)}$.

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 imbedded in a static background of impurities such that one particle with the momentum \vec{p} has a certain probability to be scattered to a new state with the momentum \vec{p} . 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

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

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 10, 8 – 10 am (Andrei Plamada, HIT E 41.2)