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 consisting of other two-state units (labeled as $\uparrow^{(R)}$ and $\downarrow^{(R)}$) and is infinitely larger than S. 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 of $\Delta \epsilon$,

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

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 beginning, 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):

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

$$\Gamma_{\uparrow\downarrow} = \Gamma w_{\downarrow}^{(R)} , \qquad \Gamma_{\downarrow\uparrow} = \Gamma w_{\uparrow}^{(R)} .$$
 (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 $P(t)^{(S)} = (N^{(S)}_{\uparrow}(t) N^{(S)}_{\downarrow}(t))/N^{(S)}$, for the following starting conditions at t = 0:
 - (i) unpolarized case $(N^{(S)}_{\uparrow} = N^{(S)}_{\downarrow}),$
 - (ii) almost complete polarization in \downarrow -direction $(N_{\downarrow}^{(S)} = N^{(S)}(1-\delta), N_{\uparrow}^{(S)} = N^{(S)}\delta, \delta \ll 1),$

(iii) almost complete polarization in \uparrow -direction $(N^{(S)}_{\uparrow} = N^{(S)}(1-\delta), N^{(S)}_{\downarrow} = N^{(S)}\delta, \delta \ll 1)$

Determine the relaxation time for these three cases. Define a temperature of the spin system $T^{(S)}$ for the three initial conditions by using a relation analogous to the definition of the temperature of the reservoir, Eq. (2).

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

The subject of this exercise is a Boltzmann equation no longer emerging from two-particle scattering, as discussed in class, but from scattering of single particles by static impurities. We assume that the particles do not interact among themselves, but are influenced by a static background of impurities which causes a particle of momentum \vec{p} to be scattered to a state with new momentum \vec{p} . We assume that the scattering happens within a negligibly short time interval and that it is elastic. Furthermore, we assume that each static scatterer is isotropic.

- a) Express these ideas mathematically: Find the relevant quantity describing the scattering, along with any of its symmetries, and write down the ensuing equation for $f(\vec{p}, \vec{p}, t)$.
- b) List all quantities conserved in the scattering and prove the conservation law

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

where $\varphi(\vec{p})$ denotes a conserved quantity.

c) State and prove the "H-theorem" for the linear Boltzmann equation. When is H constant in time? How can this H-theorem be understood physically?

Office Hours: Monday, October 5, 8-10 am (HIT K 43.2)