Tutorial sheet 5

The exercise marked with a star is homework.

Discussion topics: Green–Kubo formula; Onsager relations & fluctuation-dissipation theorem in linear response theory

14. Static linear response

Consider a system, governed by a Hamiltonian $\hat{H}_0$, at thermodynamic equilibrium at temperature T. Let $Z_0(\beta)$ and $\langle\,\cdot\,\rangle_0$ denote the corresponding (canonical) partition function and averages, with as usual $\beta = 1/k_B T$.
The system is perturbed, via a *static* modification of the Hamiltonian $\hat{H}_f = \hat{H}_0 - f\hat{A}$, leading to a new equilibrium state. The goal is to determine $\langle\hat{B}\rangle_f \equiv \mathrm{Tr}\big[\mathrm{e}^{-\beta\hat{H}_f}\hat{B}\big]/Z_f(\beta)$, where the partition function Z_f is given by $Z_f(\beta) \equiv \mathrm{Tr}\,\mathrm{e}^{-\beta\hat{H}_f}$. For that purpose, Duhamel's formula

$$\mathrm{e}^{-\beta\hat{H}} = \mathrm{e}^{-\beta\hat{H}_0} - \int_0^\beta \mathrm{e}^{-(\beta-\lambda)\hat{H}_0}\,\hat{W}\,\mathrm{e}^{-\lambda\hat{H}}\,\mathrm{d}\lambda \quad \text{for } \hat{H} = \hat{H}_0 + \hat{W} \tag{1}$$

will prove useful.

i. Compute first $Z_f(\beta)$ in function of $Z_0(\beta)$ and $\langle\hat{A}\rangle_0$ to first order in f. What does this give for the free energy of the perturbed system?

ii. Show that

$$\mathrm{Tr}\big[\mathrm{e}^{-\beta\hat{H}_f}\hat{B}\big] = Z_0(\beta)\bigg[\big\langle\hat{B}\,\big\rangle_0 + f\int_0^\beta \big\langle\hat{A}_{\mathrm{I}}(-\mathrm{i}\hbar\lambda)\,\hat{B}\,\big\rangle_0\,\mathrm{d}\lambda + \mathcal{O}(f^2)\bigg],$$

where $\hat{A}_{\mathrm{I}}(t) \equiv \mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\,\hat{A}\,\mathrm{e}^{-\mathrm{i}\hat{H}_0 t/\hbar}$ denotes the interaction-picture representation of $\hat{A}$.

iii. Deduce from the results to the first two questions the identity $\langle\hat{B}\rangle_f = \langle\hat{B}\rangle_0 + \chi_{BA}^{\text{stat.}} f + \mathcal{O}(f^2)$, where the *static response function* is given by

$$\chi_{BA}^{\text{stat.}} \equiv \int_0^\beta \Big[\big\langle\hat{A}_{\mathrm{I}}(-\mathrm{i}\hbar\lambda)\,\hat{B}\,\big\rangle_0 - \langle\hat{A}\rangle_0\langle\hat{B}\rangle_0\Big]\,\mathrm{d}\lambda.$$

Can you relate $\chi_{BA}^{\text{stat.}}$ to one of the correlation functions encountered in the lecture?

iv. If you still have time... can you prove Duhamel's formula (1)?

Hint: Find a differential equation obeyed by $\mathrm{e}^{-\beta\hat{H}}$, viewed as a function of β.

*15. Detailed balance relation

Consider a two-level system coupled to a macroscopic system Σ at thermodynamic equilibrium. The total Hamiltonian is given by

$$\hat{H} = -\frac{\hbar\omega_0}{2}\hat{\sigma}_z + \hat{H}_{\text{int}} + \hat{H}_\Sigma \equiv \hat{H}_0 + \hat{H}_{\text{int}}, \tag{2}$$

with σ_z the usual Pauli matrix and $\omega_0 > 0$. Let $|g\rangle$, $|e\rangle$ denote the two levels (ground state, excited state) of the small system and $\{\,|\phi_n\rangle\}$ be a basis of energy eigenstates of $\hat{H}_\Sigma$. The interaction between the systems is chosen so as to induce transitions in the small one:

$$\hat{H}_{\text{int}} = -\hat{\sigma}_x \otimes \hat{X}, \tag{3}$$

with $\hat{X}$ an observable of the macroscopic system.

We want to study the absorption and emission rates $\Gamma_{g\to e}$, $\Gamma_{e\to g}$ of the small system.

i. Time evolution

Let $|\psi(0)\rangle = |\alpha\rangle \otimes |\phi_n\rangle$ with $\alpha = g$ or e denote the initial state of the composite system. Check that to lowest non-trivial order in perturbation theory this state becomes at time t

$$|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}\hat{H}_0 t/\hbar}\left[1 + \frac{\mathrm{i}}{\hbar}\int_0^t \hat{\sigma}_x(t')\hat{X}(t')\,\mathrm{d}t'\right]|\psi(0)\rangle.$$

ii. Absorption rate

a) Deduce from the previous result that the absorption probability at time t when the macroscopic system is initially in the state $|\phi_n\rangle$ is given by

$$p_{\mathrm{abs}}^{(\phi_n)}(t) = \sum_m \left|\left(\langle e| \otimes \langle\phi_m|\,\right)|\psi(t)\rangle\right|^2 \simeq \frac{1}{\hbar^2}\int_0^t\int_0^t \langle\phi_n|\,\hat{X}(t')\hat{X}(t'')\,|\phi_n\rangle\,\mathrm{e}^{-\mathrm{i}\omega_0(t'-t'')}\,\mathrm{d}t'\,\mathrm{d}t''.$$

Hint: It might help to realize that $\hat{\sigma}_x(t) = \frac{1}{2}(\hat{\sigma}_+\,\mathrm{e}^{-\mathrm{i}\omega_0 t} + \hat{\sigma}_-\,\mathrm{e}^{\mathrm{i}\omega_0 t})$, from where its matrix elements become trivial, with $\sigma_\pm$ the usual linear combinations of σ_x and σ_y.

b) Check that this leads for the total absorption probability to

$$p_{\mathrm{abs}}(t) \simeq \frac{1}{\hbar^2}\int_0^t\int_0^t \left\langle\hat{X}(t')\hat{X}(t'')\right\rangle_{\mathrm{eq.}}\mathrm{e}^{-\mathrm{i}\omega_0(t'-t'')}\,\mathrm{d}t'\,\mathrm{d}t'',$$

with $\langle\,\cdot\,\rangle_{\mathrm{eq.}}$ the usual equilibrium expectation value using the density operator of the macroscopic system.

c) One recognizes in the integrand the non-symmetrized correlation function $C_{XX}(t'-t'')$ for $\hat{X}$. Assuming that this function only takes significant values when its argument is close to 0, show how you can approximate the double integral according to

$$\int_0^t\int_0^t \mathrm{d}t'\,\mathrm{d}t'' \simeq t\int_{-\infty}^{\infty}\mathrm{d}(t'-t'').$$

Deduce from there the absorption rate

$$\Gamma_{g\to e} = \frac{1}{\hbar^2}\tilde{C}_{XX}(-\omega_0), \tag{4}$$

with $\tilde{C}_{XX}$ the Fourier transform of C_{XX}.

iii. Emission rate

Repeating the computation of question **ii.** (you need not do it explicitly! the only change is that of a matrix element), deduce that the emission rate of the small system is

$$\Gamma_{e\to g} = \frac{1}{\hbar^2}\tilde{C}_{XX}(\omega_0). \tag{5}$$

iv. We let the populations π_g, π_e of the two levels according to the coupled *rate equations* (do you agree that they make sense if one remains in a linear regime?)

$$\frac{\mathrm{d}\pi_g(t)}{\mathrm{d}t} = -\Gamma_{g\to e}\pi_g(t) + \Gamma_{e\to g}\pi_e(t)$$
$$\frac{\mathrm{d}\pi_e(t)}{\mathrm{d}t} = \Gamma_{g\to e}\pi_g(t) - \Gamma_{e\to g}\pi_e(t).$$

Find the ratio π_e/π_g of these populations in the stationary regime: first in terms of the rates; then, using the **detailed balance relation** [Eq. (III.53) of the lecture notes], in terms of the energy difference between both levels. What do you recognize?

If you want more information on the possible interest of the system modeled above, you may have a look at R. J. Schoelkopf *et al.*, *Qubits as Spectrometers of Quantum Noise*, `http://arxiv.org/abs/cond-mat/0210247`.