Tutorial sheet 5

Discussion topic: linear response function and generalized susceptibility

11. Static linear response

Consider a system governed by a Hamiltonian $\hat{H}_0$, in 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, which amounts to a *static* modification of the Hamiltonian $\hat{H} = \hat{H}_0 - a\hat{A}$, leading to a new equilibrium. We wish to compute $\langle\hat{B}\rangle_a \equiv \mathrm{Tr}\big[\mathrm{e}^{-\beta\hat{H}}\,\hat{B}\big]/Z_a(\beta)$, where $Z_a(\beta) \equiv \mathrm{Tr}\,\mathrm{e}^{-\beta\hat{H}}$. 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 be exploited.

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

ii. Show that

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

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

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

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

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 show Duhamel's formula (1)?

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

12. Nonlinear response

We want to investigate the first nonlinear correction to the response of the observable $\hat{B}$ of a system in equilibrium to an external perturbation $-f(t)\hat{A}$. Writing

$$\big\langle\hat{B}(t)\big\rangle_{\text{n.eq.}} = \big\langle\hat{B}\,\big\rangle_{\text{eq.}} + \int \chi_{BA}^{(1)}(t,t')\,f(t')\,\mathrm{d}t' + \int \chi_{BA}^{(2)}(t,t',t'')\,f(t')\,f(t'')\,\mathrm{d}t'\,\mathrm{d}t'' + \mathcal{O}(f^3),$$

where the integrals run over $\mathbb{R}$, show that the nonlinearity of second order involves the response function

$$\chi_{BA}^{(2)}(t,t',t'') = \frac{1}{(\mathrm{i}\hbar)^2}\,\Theta(t-t')\,\Theta(t-t'')\,\Big\langle\Big[\big[\hat{B}(t),\hat{A}(t')\big],\hat{A}(t'')\Big]\Big\rangle_{\text{eq.}}.$$