Tutorial sheet 11

Discussion topic: linear response

22. Static linear response

Consider a system governed by a Hamiltonian $\hat{\mathsf{H}}_0$, 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 $\hat{\mathsf{H}} = \hat{\mathsf{H}}_0 - a\hat{\mathsf{A}}$, leading to a new equilibrium. We wish to compute $\langle\hat{\mathsf{B}}\rangle_a \equiv \mathrm{Tr}\big[\mathrm{e}^{-\beta\hat{\mathsf{H}}}\,\hat{\mathsf{B}}\big]/Z_a(\beta)$, where $Z_a(\beta) \equiv \mathrm{Tr}\,\mathrm{e}^{-\beta\hat{\mathsf{H}}}$. For that purpose, Duhamel's formula

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

will be exploited.

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

ii. Show that

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

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

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

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

Can you relate $\chi^{\text{stat.}}_{\mathsf{BA}}$ for $\langle\hat{\mathsf{A}}\rangle_0\langle\hat{\mathsf{B}}\rangle_0 = 0$ 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 $\mathrm{e}^{-\beta\hat{\mathsf{H}}}$, viewed as function of β.

23. Nonlinear response

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

$$\Big\langle\hat{\mathsf{B}}(t)\Big\rangle_{\text{n.eq.}} = \Big\langle\hat{\mathsf{B}}\Big\rangle_{\text{eq.}} + \int\chi^{(1)}_{\mathsf{BA}}(t,t')\,a(t')\,\mathrm{d}t' + \int\chi^{(2)}_{\mathsf{BA}}(t,t',t'')\,a(t')\,a(t'')\,\mathrm{d}t'\,\mathrm{d}t'' + \mathcal{O}(a^3),$$

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

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