Tutorial sheet 12

Discussion topic: linear response function and generalized susceptibility; Kubo formula

28. 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 $\beta = 1/k_BT$.
The system is perturbed, which amounts to 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 be exploited.

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 $\hat{A}_{\mathrm{I}}(t) \equiv \mathrm{e}^{\mathrm{i}\hat{H}_0t/\hbar}\,\hat{A}\,\mathrm{e}^{-\mathrm{i}\hat{H}_0t/\hbar}$ denotes the interaction-picture representation of $\hat{A}$.

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

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

Can you relate $\chi^{\mathrm{stat.}}_{BA}$ 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.

29. 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

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

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

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