Response and correlation functions

- **Linear response**

$$\hat{H}_{\rm tot} = \hat{H} - \int d^d r \sum_i h_i(\mathbf{r},t)\hat{A}_i(\mathbf{r})$$
$$\delta\langle \hat{A}_i(\mathbf{r},t)\rangle = \int_{-\infty}^{\infty} dt' \int d^d r' \sum_j \chi^R_{A_iA_j}(\mathbf{r},t;\mathbf{r}',t')h_j(\mathbf{r}',t') + \mathcal{O}(h_j^2) \tag{1}$$
$$\chi^R_{A_iA_j}(\mathbf{r},t;\mathbf{r}',t') = i\theta(t-t')\langle[\hat{A}_i(\mathbf{r},t),\hat{A}_j(\mathbf{r}',t')]\rangle \quad \text{("retarded" response function or susceptibility)}$$

  where $\hat{A}_i(\mathbf{r},t) = e^{i\hat{H}t}\hat{A}_i(\mathbf{r})e^{-i\hat{H}t}$ (Heisenberg representation) and $\langle\cdots\rangle = \mathrm{Tr}(e^{-\beta\hat{H}}\cdots)/\mathrm{Tr}\, e^{-\beta\hat{H}}$.

- **External field (adiabatically switched on):** $h_i(t) = h_i(\omega)e^{-i(\omega+i\eta)t} \quad (\eta\to 0^+)$

$$\delta\langle\hat{A}_i(t)\rangle = \sum_j \chi^R_{A_iA_j}(\omega)h_j(\omega)e^{-i\omega t+\eta t}, \qquad \chi^R_{A_iA_j}(\omega) = \int_{-\infty}^{\infty} dt\, \chi^R_{A_iA_j}(t)e^{i(\omega+i\eta)t} \tag{2}$$

  (To alleviate notations, we include the $\mathbf{r}$ dependence in the i index)

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$$\begin{aligned}\chi^R_{A_iA_j}(t;t') &= 2i\theta(t-t')\chi''_{A_iA_j}(t;t')\\ \chi''_{A_iA_j}(t;t') &= \frac{1}{2}\langle[\hat{A}_i(t),\hat{A}_j(t')]\rangle\end{aligned} \tag{3}$$

- **Dissipation**

$$\begin{aligned}&\overline{\frac{dW}{dt}} = \frac{1}{2}\sum_{i,j} h_i^*(\omega)\omega\chi''_{A_i^\dagger A_j}(\omega)h_j(\omega) \quad \text{(power dissipated into the system, must be positive)}\\ &\{\omega\chi''_{A_i^\dagger A_j}(\omega)\} \quad \text{positive matrix, in particular} \quad \omega\chi''_{A^\dagger A}(\omega)\geq 0\end{aligned} \tag{4}$$

- **Spectral (Lehmann) representation**

$$\begin{aligned}\chi_{A_iA_j}(z) &= \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-z} \quad (z \text{ complex frequency})\\ \chi^R_{A_iA_j}(\omega) &= \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-\omega-i\eta} = \chi_{A_iA_j}(z=\omega+i\eta)\\ \chi''_{A_iA_j}(\omega) &= \frac{\pi}{Z}\sum_{n,m}\left(e^{-\beta\epsilon_n}-e^{-\beta\epsilon_m}\right)A_i^{nm}A_j^{mn}\delta(\omega+\epsilon_n-\epsilon_m) \quad \text{(spectral function)}\end{aligned} \tag{5}$$

  where $\{|n\rangle,\epsilon_n\}$ form a complete set of eigenvectors of $\hat{H}$ and $A_i^{nm} = \langle n|\hat{A}_i|m\rangle$. $\chi_{A_iA_j}(z)$ is analytic in the whole complex plane except (possibly) on the real axis.

- $\chi''_{A^\dagger A}(\omega) = \Im[\chi^R_{A^\dagger A}(\omega)]$ is real.

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$$\chi_{A_iA_j}(z) = \frac{1}{Z}\sum_{\substack{n,m\\(\epsilon_n\neq\epsilon_m)}}\frac{e^{-\beta\epsilon_n}-e^{-\beta\epsilon_m}}{\epsilon_m-\epsilon_n-z}A_i^{nm}A_j^{mn} \tag{6}$$

- **Causality and Kramers-Kronig relations**

$$\begin{aligned}\Re[\chi^R(\omega)] &= \mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\Im[\chi^R(\omega')]}{\omega'-\omega}\\ \Im[\chi^R(\omega)] &= -\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\Re[\chi^R(\omega')]}{\omega'-\omega}\end{aligned} \tag{7}$$

- **Fluctuation-dissipation theorem**

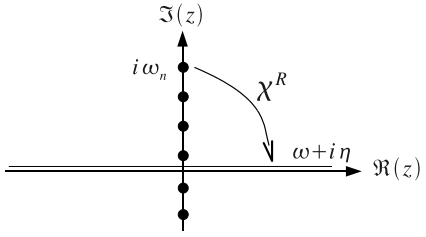
$$\begin{aligned}&S_{A_iA_j}(t) = \langle\hat{A}_i(t)\hat{A}_j\rangle - \langle\hat{A}_i\rangle\langle\hat{A}_j\rangle \quad \text{(structure factor)}\\ &\chi''_{A_iA_j}(\omega) = \frac{1}{2}\left(1-e^{-\beta\omega}\right)S_{A_iA_j}(\omega)\\ &\chi''_{A_iA_j}(\omega) = \frac{\beta\omega}{2}S_{A_iA_j}(\omega) \quad \text{i.e.} \quad \chi_{A_iA_j}(t=0) = \beta S_{A_iA_j}(t=0) \quad \text{for } |\omega| \ll T \text{ (classical limit)}\end{aligned} \tag{8}$$

- **Imaginary-time correlation functions**

$$\begin{aligned}\chi_{A_iA_j}(\tau) &= \langle T_\tau\hat{A}_i(\tau)\hat{A}_j\rangle - \langle\hat{A}_i\rangle\langle\hat{A}_j\rangle \quad \text{(imaginary-time linear response function)}\\ \chi_{A_iA_j}(i\omega_n) &= \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-i\omega_n} = \chi_{A_iA_j}(z=i\omega_n)\end{aligned} \tag{9}$$

  (the second equation is not always true for $i\omega_n = 0$) with $\hat{A}_i(\tau) = e^{\tau\hat{H}}\hat{A}_i e^{-\tau\hat{H}}$.

- **Analytic continuation**: How to obtain the retarded response function from the imaginary-time correlation function?



$$\chi^R_{A_iA_j}(\omega) = \chi_{A_iA_j}(i\omega_n \to \omega + i\eta)$$

- **One-particle Green function**: $G(\mathbf{k},\tau) = -\langle T_\tau\hat{\psi}(\mathbf{k},\tau)\hat{\psi}^\dagger(\mathbf{k},0)\rangle$

$$\begin{aligned}G(\mathbf{k},i\omega_n) &= \int_{-\infty}^{\infty}d\omega\frac{A(\mathbf{k},\omega)}{i\omega_n-\omega},\\ A(\mathbf{k},t) = \frac{1}{2\pi}\langle[\hat{\psi}(\mathbf{k},t),\hat{\psi}^\dagger(\mathbf{k},0)]_{-\zeta}\rangle, &\quad A(\mathbf{k},\omega) = -\frac{1}{\pi}\Im[G^R(\mathbf{k},\omega)],\end{aligned} \tag{10}$$

  where $\zeta = 1$ (bosons) or -1 (fermions).