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 $\langle\cdots\rangle = {\rm Tr}(e^{-\beta\hat{H}}\cdots)/{\rm Tr}\, e^{-\beta\hat{H}}$.

- **External field (adiabatically switched on)**

$$\begin{aligned} h_i(t) &= h_i(\omega)e^{-i(\omega+i\eta)t} + \text{c.c.} \quad (\eta\to 0^+) \\ \delta\langle \hat{A}_i(t)\rangle &= \sum_j \chi^R_{A_iA_j}(\omega)h_j(\omega)e^{-i\omega t+\eta t} + \text{c.c.} \\ \chi^R_{A_iA_j}(\omega) &= \int_{-\infty}^{\infty} dt\, \chi^R_{A_iA_j}(t)e^{i(\omega+i\eta)t} \end{aligned} \tag{2}$$

(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**

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

- **Spectral 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.
- **Lehmann representation**

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

- **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**

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

- **High-frequency limit**

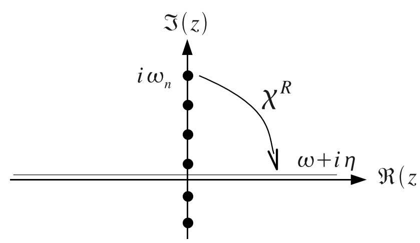
$$\begin{aligned} \chi_{A_iA_j}(z) &= -\frac{1}{z}\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \chi''_{A_iA_j}(\omega) - \frac{1}{z^2}\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega\chi''_{A_iA_j}(\omega) + \mathcal{O}\left(z^{-3}\right) \\ &= -\frac{1}{z}\langle[\hat{A}_i, \hat{A}_j]\rangle - \frac{1}{z^2}\langle[[\hat{A}_i, \hat{H}], \hat{A}_j]\rangle + \mathcal{O}\left(z^{-3}\right) \end{aligned} \tag{9}$$

- **Imaginary-time correlation functions**

$$\begin{aligned} \chi_{A_iA_j}(\tau) &= \langle T_\tau \hat{A}_i(\tau)\hat{A}_j\rangle - \langle \hat{A}_i\rangle\langle \hat{A}_j\rangle \\ \chi_{A_iA_j}(i\omega_n) &= \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_{A_iA_j}(\omega')}{\omega' - i\omega_n} = \chi_{A_iA_j}(z = i\omega_n) \end{aligned} \tag{10}$$

(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**



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

- **One-particle Green function**

$$\begin{aligned} G(\mathbf{k}, \tau) &= -\langle T_\tau \hat{\psi}(\mathbf{k}, \tau)\hat{\psi}^\dagger(\mathbf{k}, 0)\rangle \\ G(\mathbf{k}, i\omega_n) &= \int_{-\infty}^{\infty} d\omega \frac{A(\mathbf{k}, \omega)}{i\omega_n - \omega} \\ A(\mathbf{k}, t) &= \frac{1}{2\pi}\langle[\hat{\psi}(\mathbf{k}, t), \hat{\psi}^\dagger(\mathbf{k}, 0)]_{-\zeta}\rangle \\ A(\mathbf{k}, \omega) &= -\frac{1}{\pi}\Im[G^R(\mathbf{k}, \omega)] \end{aligned} \tag{11}$$

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