PJD3

LECTURE 4

Real - time GFs at finite temperature

At $T > 0$ to find neutron cross section we must take into account the thermal distribution of the initial states $|\psi_I\rangle$:

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{K}{2\pi K'}\left(\frac{M}{2\pi}\right)^2 |V_q|^2 \sum_I \int_{-\infty}^{\infty} dt\, e^{i\omega t} \sum_{j\ell} p_I \langle \psi_I | e^{-i\vec{q}\cdot\vec{X}_j(t)} e^{i\vec{q}\cdot\vec{X}_\ell(0)} | \psi_I \rangle$$

$$p_I = \frac{1}{Z(\beta)} e^{-\beta E_I} \qquad \text{Boltzman factor}$$

$$\frac{1}{Z(\beta)} \sum_I \langle \psi_I | e^{-\beta H} e^{-i\vec{q}\cdot\vec{X}_j(t)} e^{i\vec{q}\cdot\vec{X}_\ell(0)} | \psi_I \rangle$$

$$\equiv \langle e^{-i\vec{q}\cdot\vec{X}_j(t)} e^{i\vec{q}\cdot\vec{X}_\ell(0)} \rangle_\beta \qquad - \text{ thermal average}$$

$$\vec{X}_j(t) = \vec{R}_j + \vec{u}_j(t)$$

This leads to consideration of quantity

$$F(\vec{q},t) = \sum_{j\ell} e^{i\vec{q}\cdot(\vec{R}_\ell - \vec{R}_j)} \langle e^{-i\vec{q}\cdot\vec{u}_j(t)} e^{i\vec{q}\cdot\vec{u}_\ell(0)} \rangle_\beta$$

$$\simeq q^2 \sum_{j\ell} e^{i\vec{q}\cdot(\vec{R}_\ell - \vec{R}_j)} \underline{\langle u_j(t)\, u_j(0) \rangle_\beta}$$

real - time GF at nonzero T

Define: time ordered finite-T GF:

$$g_{ij}(t-t') = -i\langle T[u_i(t)\, u_j(t')]\rangle_\beta$$

$$\langle \hat{O}\rangle_\beta = \frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H}\hat{O}\right)$$

Retarded:

$$G^R_{ij}(t-t') = -i\,\theta(t-t')\langle [u_i(t), u_j(t')]\rangle_\beta$$

Analytic continuation

- key result derived in Appendix 2 of the textbook.
- every aspiring theorist in the class should go through this derivation.

• Relates $G^R_{ij}(t-t')$ to $g_{ij}(\tau-\tau')$ via "spectral representation"

$$\boxed{\begin{aligned} G^R_{ij}(\omega) &= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left(1-e^{-\beta\omega'}\right)\frac{A_{ij}(\omega')}{\omega-\omega'+i\varepsilon} \qquad (+) \\ g_{ij}(\omega_n) &= -\frac{1}{\beta}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left(1-e^{-\beta\omega'}\right)\frac{A_{ij}(\omega')}{-i\omega_n-\omega'} \end{aligned}}$$

$$\boxed{G^R_{ij}(\omega) = -\beta\, g_{ij}(i\omega-\varepsilon)} \leftarrow \text{analytic continuation}$$

Here $A_{ij}(\omega)$ is the "spectral function" (or "spectral density") given by

$$\boxed{\begin{aligned} A_{ij}(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle u_i(t)\, u_j(0) \rangle_\beta \\ &= \frac{2\pi}{Z(\beta)} \sum_{mn} e^{-\beta E_m} \langle n | u_i | m \rangle \langle m | u_j | n \rangle\, \delta(E_m - E_n + \omega) \end{aligned}}$$

Lehmann representation

Note that when $i = j$ ~~(which is usually the case of interest)~~ $A_{ii}(\omega)$ is real and non-negative.

For phonons we previously derived $g_k(\omega_n) = \frac{1}{\beta M} \frac{1}{\omega_n^2 + \Omega_k^2}$ so we get immediately:

$$\boxed{\begin{aligned} G_k^R(\omega) &= -\frac{1}{M} \cdot \frac{1}{-(\omega + i\varepsilon)^2 + \Omega_k^2} \\ &= \frac{1}{2M\Omega_k} \left(\frac{1}{\omega - \Omega_k + i\varepsilon} - \frac{1}{\omega + \Omega_k + i\varepsilon} \right) \end{aligned}}$$

- One can obtain $A_k(\omega)$ from $G_k^R(\omega)$ by inverting Eq. (+)

$$A_k(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle u_k(t)\, u_k(0) \rangle_\beta \quad \text{- Real (see Lehman representation)}$$

Use the formula
$$\frac{1}{x+i\epsilon} = \mathcal{P}\frac{1}{x} - i\pi\delta(x)$$

principal part

$$G_k^R(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left(1-e^{-\beta\omega'}\right)A_k(\omega)\left[\mathcal{P}\frac{1}{\omega-\omega'} - i\pi\delta(\omega-\omega')\right]$$

$$\mathrm{Im}\, G_k^R(\omega) = -\frac{1}{2}\left(1-e^{-\beta\omega}\right)A_k(\omega)$$

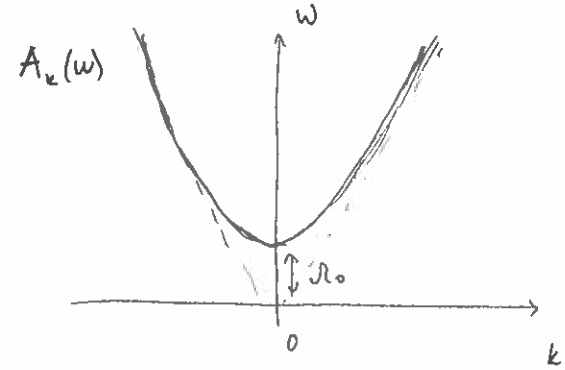
$$\boxed{A_k(\omega) = \frac{2}{1-e^{-\beta\omega}}\,\mathrm{Im}\, G^R(\omega)}$$

holds generally
[whenever $A_k(\omega)$ is real]

$$= \frac{\pi}{M\Omega_k\left(1-e^{-\beta\omega}\right)}\left[\delta(\omega-\Omega_k)-\delta(\omega+\Omega_k)\right]$$

Physical meaning: $\Omega_k = \sqrt{\Omega_0^2 + D_k} \geq 0$ energy dispersion of the phonon

suppose $D_k \simeq v^2 k^2$



$$A_k(\omega) = \frac{2\pi}{Z(\beta)}\sum_{n,m} e^{-\beta E_m}\left|\langle n|u_k|m\rangle\right|^2\delta(E_m-E_n+\omega)$$

$A_k(\omega)$ contains full information about the excitation spectrum AND some information about the wave functions

— see p. 43-44 for relation to neutron scattering

THE FEYNMAN - DYSON EXPANSION

(Systematics of Feynman diagrams.)

1. The interaction picture

$$H = H_0 + H_1$$

Schrödinger picture	Interaction picture	Heisenberg picture
$i\frac{\partial\lvert\Psi_s\rangle}{\partial t} = H\lvert\Psi_s\rangle$ $\hat{O}_s$ - time indep.	$i\frac{\partial\lvert\Psi_I\rangle}{\partial t} = H_1(t)\lvert\Psi_I\rangle$ $O_I(t) = e^{iH_0t}O_s e^{-iH_0t}$	$\lvert\Psi_H\rangle$ - time indep $i\frac{\partial\hat{O}_H}{\partial t} = [H, \hat{O}_H]$

$$H_1(t) = e^{iH_0t} H_1 e^{-iH_0t}$$

- Evolution of states is given by time-evolution operator

$$\lvert\Psi_I(t)\rangle = e^{iH_0t}\lvert\Psi_s(t)\rangle \equiv U(t,t')\lvert\Psi_I(t')\rangle \leftarrow$$

$$\lvert\Psi_s(t)\rangle = e^{iHt}\lvert\Psi_s(0)\rangle$$

$$\Rightarrow \quad U(t,t') = e^{iH_0t}e^{-iH(t-t')}e^{-iH_0t'}$$

Operator $U(t,t')$ satisfies Eq. of motion

$$i\frac{\partial U(t,t')}{\partial t} = H_1(t)\,U(t,t') \qquad \text{(check !)}$$

~~and~~ the "group property",

$$U(t,t')\,U(t',t'') = U(t,t'') \qquad \text{(check !)}$$

and

$$U(t,t') = U(t',t)^{+},$$

$$U(t,t')\,U(t,t')^{+} = 1 \qquad \text{(check !)}$$

Relation between Interaction and Heisenberg pictures

$$|\Psi_H\rangle = e^{iHt}\,|\Psi_s(t)\rangle = e^{iHt}e^{-iH_0t}\,|\Psi_I(t)\rangle = U(t,0)^{+}|\Psi_I(t)\rangle$$

$$O_H(t) = U^{+}(t,0)\,O_I(t)\,U(t,0)$$

Some comments on the spectral function

$$A_k(\omega) = \frac{\pi}{M\Omega_k(1-e^{-\beta\omega})}\left[\delta(\omega-\Omega_k) - \delta(\omega+\Omega_k)\right] \qquad \Omega_k = \sqrt{\Omega_0^2 + D_k}$$

$T \to 0$ ($\beta \to \infty$) limit

$$\frac{1}{1-e^{-\beta\omega}} \longrightarrow \begin{cases} 1 & \omega > 0 \\ 0 & \omega < 0 \end{cases} \qquad A_k(\omega) = \frac{\pi}{M\Omega_k}\delta(\omega-\Omega_k)$$

$T \to \infty$ ($\beta \to 0$) limit

$e^{-\beta\omega} \to 1$, $\frac{1}{1-e^{-\beta\omega}} \to \infty$ for any ω.

This is interpreted simply as the # of phonons per unit volume of the crystal <u>diverging</u> at any energy.

The sum rule

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi} A_k(\omega) = \frac{1}{2M\Omega_k}\left[\frac{1}{1-e^{-\beta\Omega_k}} - \frac{1}{1-e^{\beta\Omega_k}}\right]$$

$$= \frac{1}{2M\Omega_k}\left[\frac{1}{1-e^{-\beta\Omega_k}} - \frac{e^{-\beta\Omega_k}}{e^{-\beta\Omega_k}-1}\right]$$

$$= \frac{1}{2M\Omega_k}\,\frac{1+e^{-\beta\Omega_k}}{1-e^{-\beta\Omega_k}} = \frac{1}{2M\Omega_k}\coth\tfrac{1}{2}\beta\Omega_k$$