2. GF at finite temperatures

At non-zero T we consider free energy $(\beta = 1/k_B T)$

$$Z(\beta) = e^{-\beta \mathcal{F}(\beta)} = \sum_n e^{-\beta E_n(\lambda)} \quad \Rightarrow \quad -\beta \mathcal{F} = \ln \sum_n e^{-\beta E_n(\lambda)}$$

where $E_n(\lambda)$ are energy eigenvalues of $H(\lambda) = H_0 + \lambda H_1$:

$$H(\lambda)\,|\Psi_n(\lambda)\rangle = E_n(\lambda)\,|\Psi_n(\lambda)\rangle .$$

- We can perform similar manipulation that led to ΔE_G

$$\frac{\partial \mathcal{F}}{\partial \lambda} = \frac{\sum_n e^{-\beta E_n(\lambda)} \frac{\partial E_n(\lambda)}{\partial \lambda}}{\sum_n e^{-\beta E_n(\lambda)}} = \frac{\sum_n e^{-\beta E_n(\lambda)} \langle \Psi_n(\lambda) | H_1 | \Psi_n(\lambda) \rangle}{Z(\beta)}$$

$$\equiv \langle H_1 \rangle_\beta \leftarrow \underline{\text{thermal average of } H_1}$$

Sometimes it is useful to write

$$\boxed{\begin{aligned} \langle \hat{O} \rangle_\beta &= \frac{1}{Z} \sum_n e^{-\beta E_n} \langle \Psi_n | \hat{O} | \Psi_n \rangle \\ &= \frac{1}{Z} \sum_n \langle \Psi_n | e^{-\beta H} \hat{O} | \Psi_n \rangle \\ &= \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H} \hat{O} \right) \end{aligned}}$$

"thermal density matrix" $\hat{\rho}_\beta \equiv e^{-\beta H}$

- In the same way we found expression for ΔE_G we now get

$$\Delta \mathcal{F} = \frac{1}{2} M \sum_{i \neq j} D_{ij} \int_0^{\lambda} d\lambda \, \langle u_i u_j \rangle_\beta$$

This motivates definition of a THERMAL or MATSUBARA Green's function

$$\boxed{g_{ij}(\tau, \tau') = \langle T_\tau [\tilde{u}_i(\tau) \tilde{u}_j(\tau')] \rangle_\beta} = g_{ij}(\tau - \tau')$$

$$\boxed{\tilde{u}(\tau) = e^{\tau H} u \, e^{-\tau H}}$$ "modified Heisenberg operator"

τ - "imaginary time"

satisfies:

$$\frac{\partial \tilde{u}(\tau)}{\partial \tau} = [H, \tilde{u}]$$

$$\langle u_i u_j \rangle_\beta = \lim_{\tau \to 0^+} g_{ij}(\tau)$$

Matsubara GF satisfies Eq of motion

$$\left(\frac{d^2}{d\tau^2} - \Omega_0^2 \right) g_{ij}(\tau) = -\frac{1}{M} \delta_{ij} \delta(\tau) + \lambda \sum_{\ell} D_{i\ell} g_{\ell j}(\tau)$$

Unperturbed GF $g^0_{ij}(\tau) = \delta_{ij} g^0(\tau)$ satisfies

$$\left(\frac{d^2}{d\tau^2} - \Omega_0^2 \right) g^0(\tau) = -\frac{1}{M} \delta(\tau)$$

and is solved by

$$\boxed{g^0(\tau) = \frac{1}{2M\Omega_0}\left[(n_0+1)\,e^{-\Omega_0|\tau|} + n_0\,e^{\Omega_0|\tau|}\right]}$$

(see p. 36 for derivation)

$$n_0 = \frac{1}{e^{\beta\Omega_0}-1}$$ Bose-Einstein distribution function

• Fundamental Periodicity property of $g(\tau)$ in imaginary time

Consider $$g_{ij}(\tau) = \langle T_\tau [u_i(\tau)\, u_j(0)]\rangle_\beta \qquad 0 \le \tau < \beta$$

$$= \frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H} u_i(\tau)\, u_j(0)\right]$$

(cyclic property of the trace)

$$= \frac{1}{Z}\,\mathrm{Tr}\left[\ u_j(0)\, e^{-\beta H} u_i(\tau)\right]$$

insert $\mathbb{1} = e^{-\beta H} e^{\beta H}$

$$= \frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H}\left(e^{\beta H} u_j(0)\, e^{-\beta H}\right) u_i(\tau)\right]$$

$$= \frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H}\ u_j(\beta)\, u_i(\tau)\right]$$

$$= \frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H}\ T_\tau\left[u_i(\tau)\, u_j(\beta)\right]\right] \equiv g_{ij}(\tau-\beta)$$

$\Rightarrow$ $g_{ij}(\tau)$ is a PERIODIC function of τ with a fundamental domain $\tau \in (0,\beta)$ and

$$g_{ij}(\tau + n\beta) = g_{ij}(\tau), \qquad n = \pm 1, \pm 2, \ldots$$

Because of the τ-periodicity the frequency-space description involves discrete "Matsubara" frequencies

$$\boxed{g(\tau) = \sum_n e^{i\omega_n \tau} g(\omega_n) \qquad \omega_n = \frac{2\pi}{\beta} n \, , \quad n = 0, \pm 1, \ldots}$$

Cleary $g(\tau+\beta) = g(\tau)$.

- Inverse transf: $\boxed{g(\omega_n) = \frac{1}{\beta} \int_0^\beta d\tau \, e^{-i\omega_n \tau} g(\tau)}$

Find $g^0(\omega_n)$

$$g^0(\tau) = \frac{1}{2M\Omega_0} \left[(n_0+1) e^{-\Omega_0 \tau} + n_0 e^{\Omega \tau} \right] \quad 0 \le \tau < \beta$$

$$g^0(\omega_n) = \frac{1}{2M\Omega_0\beta} \int_0^\beta d\tau \, e^{-i\omega_n \tau} \left[(n_0+1) e^{-\Omega_0 \tau} + n_0 e^{\Omega \tau} \right]$$

$$= \frac{1}{2M\Omega_0\beta} \left[\frac{1}{i\omega_n + \Omega_0} - \frac{1}{i\omega_n - \Omega_0} \right] = \frac{1}{\beta M} \frac{1}{\omega_n^2 + \Omega_0^2}$$

Calculate the full $g_{ij}(\omega_n)$ using the same method as for $G_{ij}(\omega)$ before:

$$g_{ij}(i\omega_n) = g^0(i\omega_n) \delta_{ij} - \lambda \beta M g^0(i\omega_n) \sum_e D_{ie} g_{ej}(i\omega_n)$$

$$\rightarrow \quad g_k(i\omega_n) = \frac{g^0(i\omega_n)}{1 + \lambda\beta M g^0(i\omega_n) D_k} = \frac{1}{\beta M} \frac{1}{\omega_n^2 + \Omega_k^2}$$

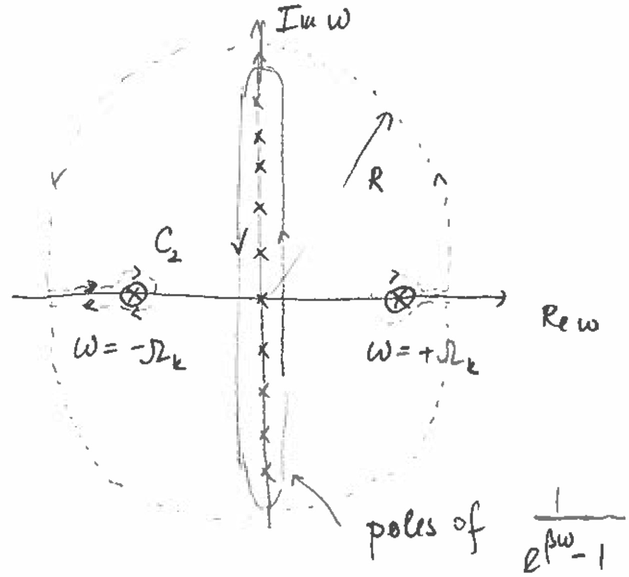
$$\Omega_k^2 = \Omega_0^2 + \lambda D_k$$

Evaluation of $\Delta\mathcal{F}$ and the Matsubara sums

$$\Delta\mathcal{F} = \frac{1}{2}\frac{M}{N}\sum_{i\neq j} D_{ij}\sum_{k} e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)}\int_0^1 d\lambda \lim_{\tau\to 0^+}\sum_n e^{i\omega_n\tau} g_k(\omega_n)$$

$$= \frac{1}{2}M \lim_{\tau\to 0^+}\int_0^1 d\lambda \sum_k D_k \underbrace{\sum_n e^{i\omega_n\tau} g_k(\omega_n)}_{\text{"Matsubara sum"}} \qquad \omega_n = \frac{2\pi}{\beta}n$$

Computation of Matsubara sums by contour integration



Take $0\le\tau\le\beta$ and write

$$g_k(\tau) = \sum_n e^{i\omega_n\tau} g_k(\omega_n)$$

$$= \frac{\beta}{2\pi i}\oint_{C_1} d\omega \frac{e^{\tau\omega}}{e^{\beta\omega}-1} g_k(i\omega)$$

$$g_k(i\omega) = \frac{1}{\beta M}\frac{1}{(i\omega)^2+\Omega_k^2} = -\frac{1}{2\Omega_k\beta M}\left[\frac{1}{\omega+\Omega_k} - \frac{1}{\omega-\Omega_k}\right]$$

$$e^{\beta\omega} = 1$$
$$\beta\omega = 2\pi i n$$
$$\omega_n = \frac{2\pi i}{\beta}n$$

Deform the contour to C_2:

$$g_k(\tau) = \frac{\beta}{2\pi i}\oint_{C_2} d\omega \frac{e^{\tau\omega}}{e^{\beta\omega}-1} g_k(i\omega)$$

$$= \frac{1}{2\Omega_k M}\left[\frac{e^{\tau\Omega_k}}{e^{\beta\Omega_k}-1} - \frac{e^{-\tau\Omega_k}}{e^{-\beta\Omega_k}-1}\right] \xrightarrow{\tau\to 0^+} \frac{1}{2\Omega_k M}\coth\frac{1}{2}\beta\Omega_k$$

$$\Omega_k = \sqrt{\Omega_0^2 + \lambda D_k}$$

Need to perform $\int_0^1 d\lambda$

Notice that:

$$\frac{\partial}{\partial \lambda} \ln \left[\sinh \tfrac{1}{2} \beta \Omega_k \right] = \frac{\beta D_k}{4 \Omega_k} \coth \tfrac{1}{2} \beta \Omega_k$$

So: $$\Delta \mathcal{F} = \tfrac{1}{2} M \int_0^1 d\lambda \sum_k D_k \frac{1}{2 \Omega_k M} \coth \left(\tfrac{1}{2} \beta \Omega_k \right)$$

$$= \frac{1}{\beta} \sum_k \ln \left[\frac{\sinh \left(\frac{1}{2} \beta \Omega_k \right)}{\sinh \left(\frac{1}{2} \beta \Omega_0 \right)} \right]$$