FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

1º Semestre de 2025

12/06/2025

Aula 25

Aulas passadas

Funções de Green de Matsubara: frequências de Matsubara

$$\mathcal{G}_{\alpha\beta}\left(\boldsymbol{r}_1,\boldsymbol{r}_2,\tau\right) = T\sum_{\omega_n} e^{-i\omega_n\tau}\mathcal{G}_{\alpha\beta}\left(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega_n\right),$$

$$\mathcal{G}_{\alpha\beta}\left(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega_n\right) = \int_0^\beta d\tau e^{i\omega_n\tau}\mathcal{G}_{\alpha\beta}\left(\boldsymbol{r}_1,\boldsymbol{r}_2,\tau\right),$$

$$\omega_n = 2\pi nT \;\; (n=0,\pm1,\pm2,\ldots) \;\; (\text{bósons}),$$

$$\omega_n = (2n+1)\,\pi T \;\; (n=0,\pm1,\pm2,\ldots) \;\; (\text{férmions}).$$

Funções de Green de Matsubara: caso não interagente

$$\widehat{H}_0 = \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}a^\dagger_{\mathbf{k},\sigma}a_{\mathbf{k},\sigma} \qquad \mathcal{G}^{(0)}_{\alpha\beta}\left(\mathbf{k},i\omega_n\right) = \frac{\delta_{\alpha,\beta}}{i\omega_n-\epsilon_{\mathbf{k}}}$$

válida para férmions ou bósons.

Aulas passadas

$$\rho(\mathbf{k},\omega) = \frac{1}{(2s+1)\,Z}\sum_{m,n}\left\{e^{-\beta K_m}(2\pi)^4\,\delta\left[\omega-(K_n-K_m)\right]\delta^{(3)}\left[\mathbf{k}-(\mathbf{P}_n-\mathbf{P}_m)\right]\right.$$
$$\left.\left(1-\zeta e^{-\beta\omega}\right)\left|\langle m|\,\psi_\alpha(0)\,|n\rangle\right|^2\right\} \qquad (K_n = E_n - \mu N_n)$$

$$\boxed{\begin{aligned}\zeta &= 1 \text{ (bósons)}\\ \zeta &= -1 \text{ (férmions)}\end{aligned}}$$

$$G^R(\mathbf{k},\omega) = \int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\frac{\rho(\mathbf{k},\omega')}{\omega-\omega'+i\eta}$$

$$G^A(\mathbf{k},\omega) = \int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\frac{\rho(\mathbf{k},\omega')}{\omega-\omega'-i\eta}$$

$$\mathcal{G}(\mathbf{k},i\omega_n) = \int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\frac{\rho(\mathbf{k},\omega')}{i\omega_n-\omega'}$$

$$\boxed{\Gamma(\mathbf{k},z) = \int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\frac{\rho(\mathbf{k},\omega')}{z-\omega'}}$$

$$G(\mathbf{k},\omega) = \left[1+\zeta f_\zeta(\omega)\right]G^R(\mathbf{k},\omega) - \zeta f_\zeta(\omega)\,G^A(\mathbf{k},\omega)$$

$$f_\zeta(\omega) = \frac{1}{e^{\beta\omega}-\zeta}$$

Aula passada

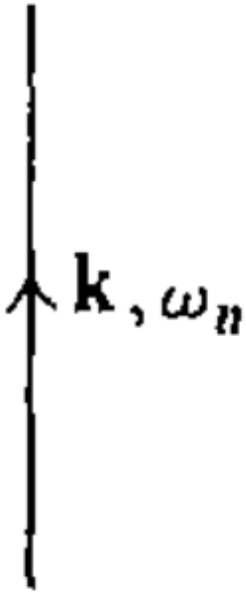
1. Draw all topologically distinct connected graphs with n interaction lines and $2n + 1$ directed particle lines.
2. Assign a direction to each interaction line. Associate a wave vector and discrete frequency with each line and conserve each quantity at every vertex.
3. With each particle line associate a factor

$$\mathcal{G}^0_{\alpha\beta}(\mathbf{k},\omega_m) = \frac{\delta_{\alpha\beta}}{i\omega_m - \hbar^{-1}(\epsilon^0_k - \mu)} \tag{25.28}$$

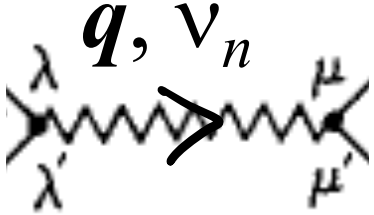
   where ω_m contains even (odd) integers for bosons (fermions).
4. Associate a factor $\mathcal{V}_0(\mathbf{k},\omega_m) \equiv V(\mathbf{k})$ with each interaction line.
5. Integrate over all n independent internal wave vectors and sum over all n independent internal frequencies.
6. The indices form a matrix product along any continuous particle line. Evaluate all matrix sums.
7. Multiply by $[-\beta\hbar^2(2\pi)^3]^{-n}(-1)^F$, where F is the number of closed fermion loops.
8. Whenever a particle line either closes on itself or is joined by the same interaction line, insert a convergence factor $e^{i\omega_m\eta}$.

Aula passada

Elementos dos diagramas



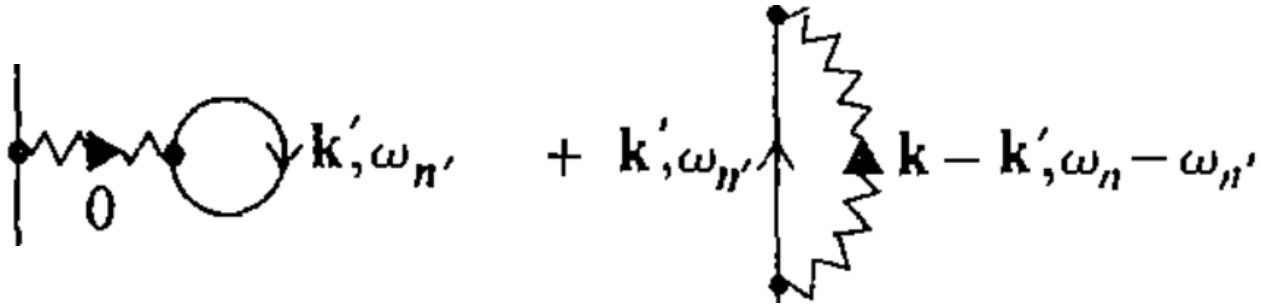
$$-\mathcal{G}^{(0)}_{\alpha\beta}\left(\mathbf{k}, i\omega_n\right) = -\frac{\delta_{\alpha,\beta}}{i\omega_n - \epsilon_{\mathbf{k}}}$$



$$-U\left(\mathbf{q}\right)\delta_{\lambda,\lambda'}\delta_{\mu,\mu'}$$

Aula passada

Auto-energia em 1ª ordem:



$$\Sigma^{(1)}\left(\mathbf{k}, i\omega_n\right) = -T\sum_{\omega_n'}\int \frac{d^3k'}{(2\pi)^3} e^{i\omega_n'\eta}\mathcal{G}^{(0)}\left(\mathbf{k}', i\omega_n'\right)\left[V\left(\mathbf{k}-\mathbf{k}'\right) + \zeta\left(2s+1\right)V\left(\mathbf{0}\right)\right]$$

$$T\sum_{\omega_n} e^{i\omega_n\eta}\mathcal{G}^{(0)}\left(\mathbf{k}, i\omega_n\right) = T\sum_{\omega_n}\frac{e^{i\omega_n\eta}}{i\omega_n - \epsilon_{\mathbf{k}}} \equiv H(\epsilon_{\mathbf{k}})$$

Cálculo de somas de Matsubara

$$H(x) = T\sum_{\omega_n} \frac{e^{i\omega_n \eta}}{i\omega_n - x}$$

DEFINO A FUNÇÃO:

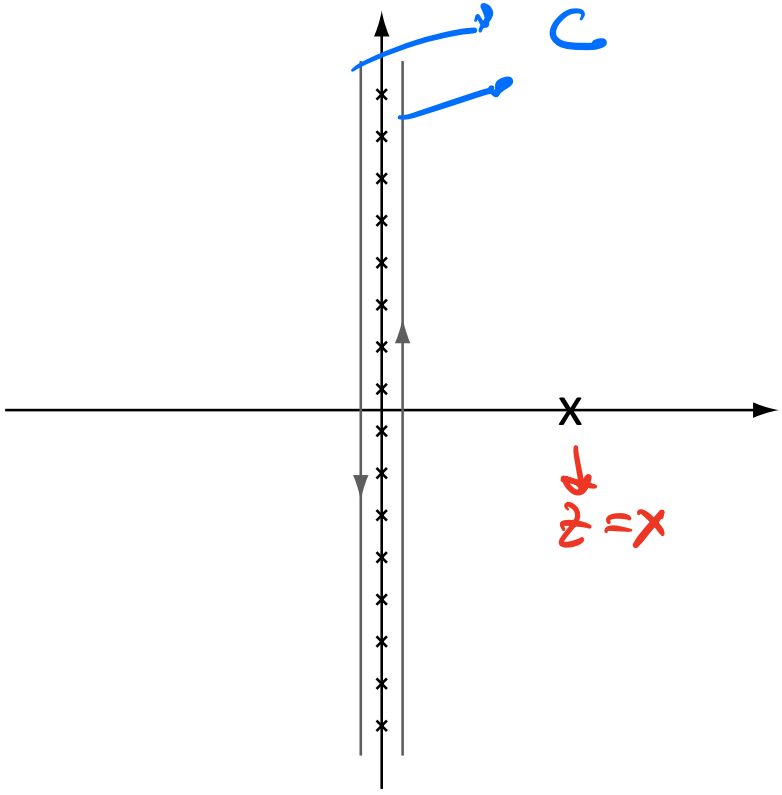
$$\bar{f}_\zeta(z) = \frac{\zeta\beta}{e^{\beta z} - \zeta} = \begin{cases} \dfrac{\beta}{e^{\beta z}-1} & \zeta = 1 \ (B) \\ \dfrac{-\beta}{e^{\beta z}+1} & \zeta = -1 \ (F) \end{cases}$$

A FUNÇÃO $\bar{f}_\zeta(z)$:

(i) POLOS SIMPLES:

$$e^{\beta z} = \zeta \Rightarrow \begin{cases} \beta z_n = 2\pi n i \ ; & \zeta = 1 \\ \beta z_n = (2n+1)\pi i \ ; & \zeta = -1 \end{cases}$$

$$\Rightarrow \boxed{z_n = i\omega_n}$$



DERIVADA DE $e^{\beta z} - \zeta$ EM z_n:

$= \beta e^{\beta z_n} = \zeta\beta \neq 0 \Rightarrow$ POLO SIMPLES

COM RESÍDUO: $\dfrac{\zeta\beta}{\frac{\partial}{\partial z}(e^{\beta z} - \zeta)\Big|_{z_n}} = 1$

PORTANTO:

$$H(x) = \int_C \frac{dz}{2\pi i} \frac{e^{\eta z}}{z - x} \frac{\beta}{e^{\beta z} - \zeta} = \cancel{2\pi i} \sum_{RQs} \frac{1}{\cancel{2\pi i}} \frac{e^{\eta z_n}}{z_n - x} = H(x)$$

DE MANEIRA GERAL:

$$G(x) = T \sum_{\omega_n} g(\omega_n) = \int_C \frac{dz}{2\pi i} g(z) \frac{\beta}{e^{\beta z} - \zeta}$$

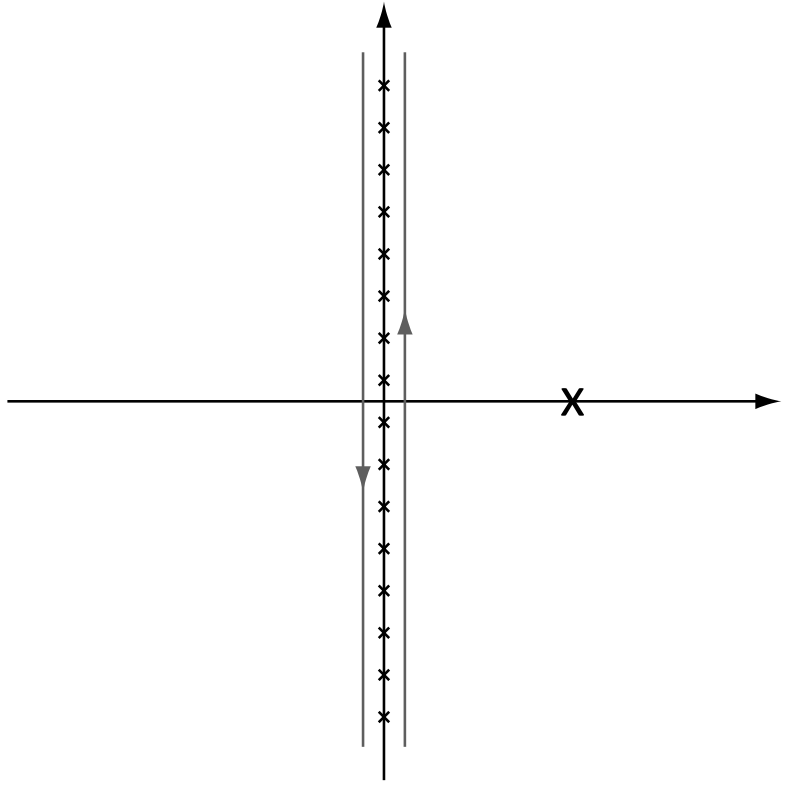
COMO CALCULAR A INTEGRAL AO LONGO DE C

Cálculo de somas de Matsubara

$$H(x) = T\sum_{\omega_n} \frac{e^{i\omega_n \eta}}{i\omega_n - x} \qquad \begin{aligned} \omega_n &= 2\pi n T \ \ (n = 0, \pm 1, \pm 2, \ldots), \\ \omega_n &= (2n+1)\pi T \ \ (n = 0, \pm 1, \pm 2, \ldots). \end{aligned}$$

$$f(z) = \frac{\zeta\beta}{e^{\beta z} - \zeta} \Rightarrow \text{ Polos simples em } z_n = i\omega_n \text{ com resíduo } 1$$

$$H(x) = T\int_C \frac{dz}{2\pi i}\left(\frac{\zeta\beta}{e^{\beta z} - \zeta}\right)\left(\frac{e^{z\eta}}{z - x}\right)$$

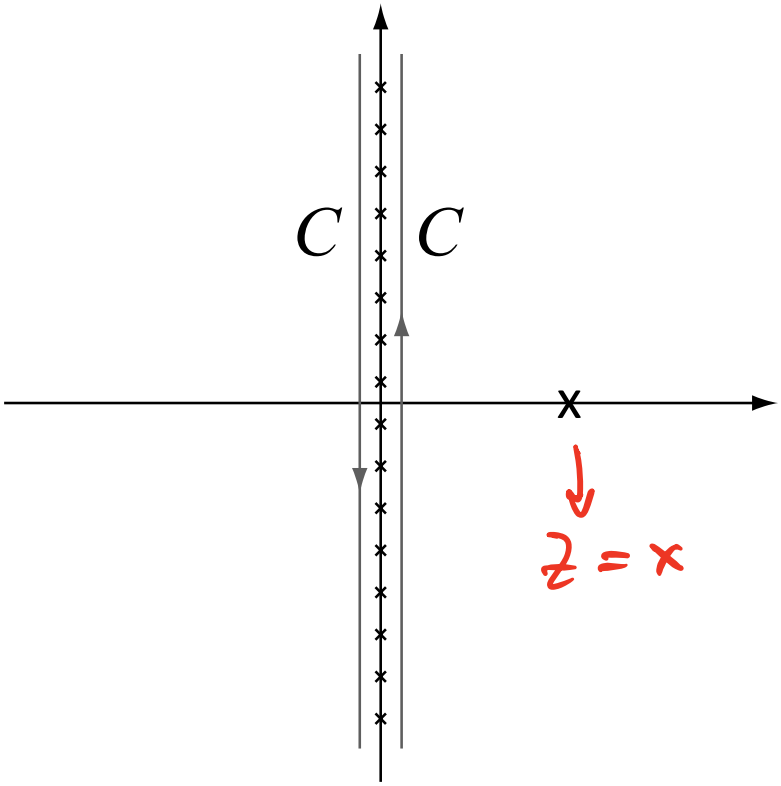


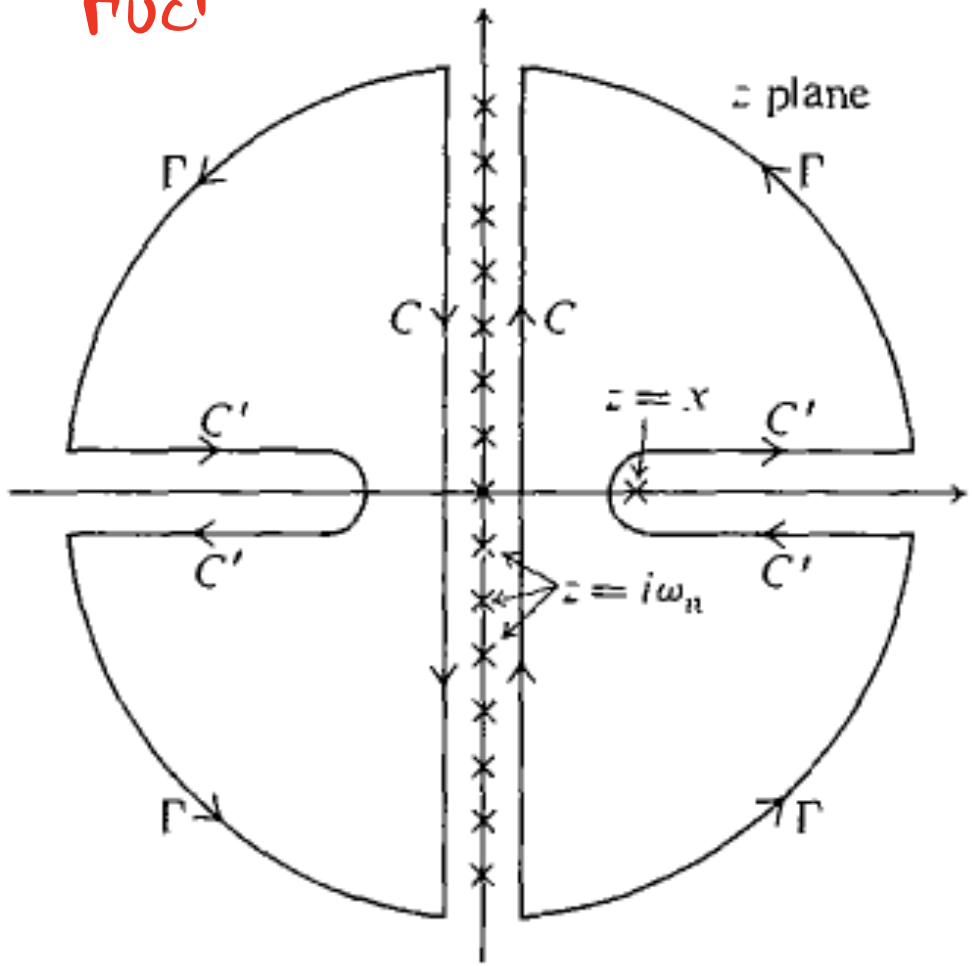
De maneira geral:

$$T\sum_{\omega_n} A(\omega_n) = T\int_C \frac{dz}{2\pi i}\left(\frac{\zeta\beta}{e^{\beta z} - \zeta}\right) A(z)$$

Cálculo de somas de Matsubara

$$H(x) = T\int_C \frac{dz}{2\pi i}\left(\frac{\zeta\beta}{e^{\beta z}-\zeta}\right)\left(\frac{e^{z\eta}}{z-x}\right) = T\int_{\Gamma\cup C'} \frac{dz}{2\pi i}\left(\frac{\zeta\beta}{e^{\beta z}-\zeta}\right)\frac{e^{\eta z}}{z-x}$$



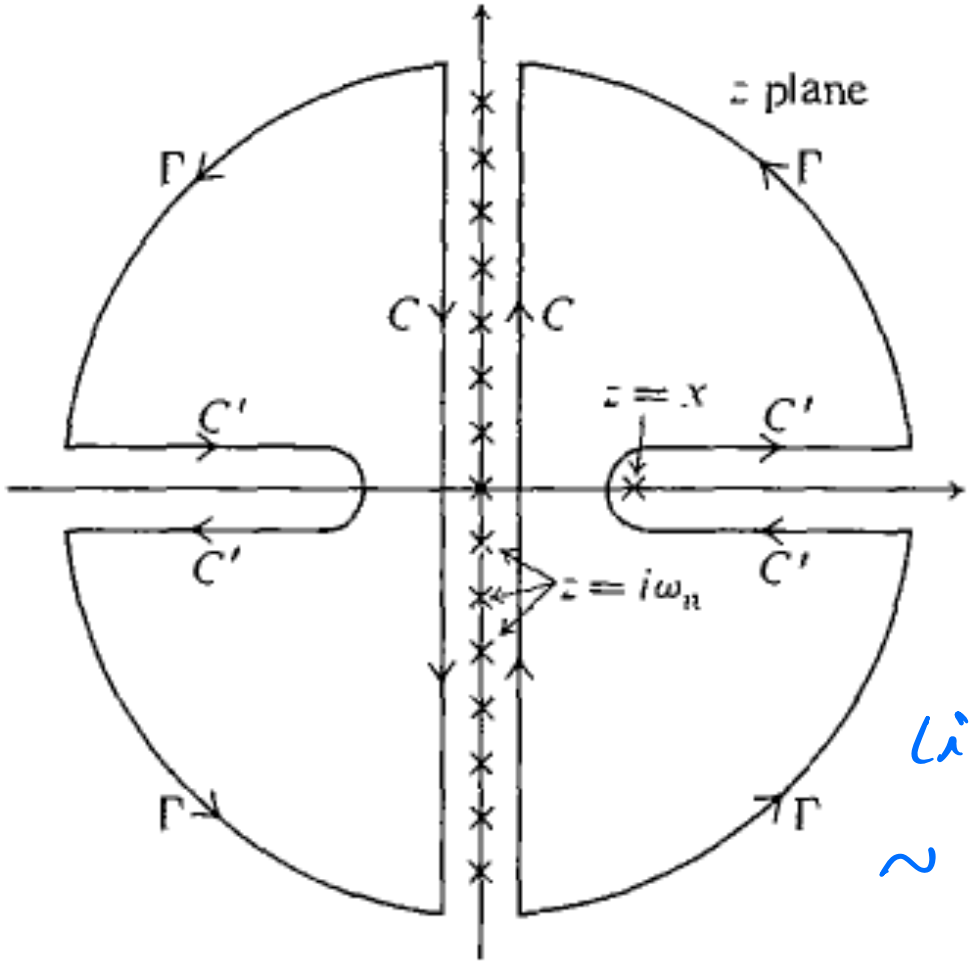


Deforma-se o caminho original C em Γ U C'

Cálculo de somas de Matsubara

$$H(x) = \int_{\Gamma \cup C'} \frac{dz}{2\pi i} \left(\frac{\zeta\beta}{e^{\beta z} - \zeta} \right) \left(\frac{e^{z\eta}}{z - x} \right)$$

VAMOS PROVAR QUE A CONTRIBUIÇÃO DE Γ É NULA:



(i) SEMI-CÍRCULO NA REGIÃO $\mathrm{Re}\, z > 0$ →

AO LONGO DESSE SEMI-CÍRCULO DE RAIO $R \to \infty$, O INTEGRANDO

$$\sim \frac{e^{(\eta-\beta)Re^{i\theta}}}{Re^{i\theta}} \qquad \theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$$

$$\xrightarrow[R\to\infty]{} e^{-\beta R} \to 0$$

(ii) SEMI-CÍRCULO C

$$\sim \frac{e^{\eta z}}{R} \xrightarrow[R\to\infty]{} 0$$

COMO A INTEGRAL SOBRE $\Gamma \to 0$, RESTA A CONTRIBUIÇÃO DE C':

$$H(x) = \int_{C'} \frac{dz}{2\pi i} \left(\frac{1}{e^{\beta z} - 1} \right) \frac{e^{\eta z}}{z - x}$$

$$= -2\pi i \sum_{\substack{\text{RES} \\ \text{EM} \\ z = x}} \text{INTEGRANDO} = -\frac{1}{e^{\beta x} - 1} e^{\eta x} \xrightarrow[\eta \to 0^+]{} -\frac{1}{e^{\beta x} - 1}$$

$$= -1 \, f_1(x) = \begin{cases} -\dfrac{1}{e^{\beta x} - 1} & (B) \\ \dfrac{1}{e^{\beta x} + 1} & (F) \end{cases}$$

$$\Rightarrow \Sigma^{(1)}(\omega_n, \vec{k}) = \int \frac{d^3 q}{(2\pi)^3} \frac{1}{e^{\beta \epsilon_q} - 1} \left[V(\vec{k} - \vec{q}) + 1 \, V(\vec{0}) \, (2S+1) \right]$$

$$V \int \frac{d^3 q}{(2\pi)^3} \frac{1}{e^{\beta \epsilon_q} - 1} = \langle \hat{N} \rangle = N$$

PORQUE O POT. QUÍM. μ É O DO SIST. INT.

Resposta linear a temperatura finita

$H(t) = H + H_{ext}(t)$ $\qquad H_{ext}(t) = 0 \quad t < t_0$

VIMOS QUE, PARA UM OBSERVÁVEL B:

$$\delta \langle \bar{\Psi}'_s(t) | B | \bar{\Psi}_s(t) \rangle = i \int_{t_0}^{t} dt' \langle \Psi'_H | \left[H_{ext\,H}(t'), B_H(t) \right] | \Psi_H \rangle$$

PARA UM ESTADO GENÉRICO $|jN\rangle$ DO SETOR DE N PARTÍCULAS:

$$\delta \langle jN(t) | B | jN(t) \rangle = i \int_{t_0}^{t} dt' \langle jN_H | \left[H_{ext,H}(t'), B_H(t) \right] | jN_H \rangle$$

TOMANDO TRAÇO NO GRANDE-CANÔNICO $\sum_{jN}$:

$$\delta \langle B \rangle(t) = i \int_{t_0}^{t} dt' \, Tr \left[\frac{e^{-\beta H}}{\Xi} \left[H_{ext,H}(t'), B_H(t) \right] \right]$$

↳ RESPOSTA LINEAR A $T \neq 0$.

PARA UMA PERTURBAÇÃO: $H_{ext}(t) = \int d^3x\, A(\vec{x})\, \phi(\vec{x},t)$

E MEDINDO $B(\vec{x})$:

$$\delta\langle B(\vec{x},t)\rangle = -i \int_{t_0}^{t} dt' \int d^3x'\, T_\Lambda \left\{ \frac{\rho}{2} \left[B_H(\vec{x},t), A_H(\vec{x}',t') \right] \right\} \phi(\vec{x}',t')$$

$$= \int_{-\infty}^{+\infty} dt' \int d^3x'\, D_{BA}(\vec{x},t;\vec{x}',t')\, \phi(\vec{x}',t')$$

ONDE:

$$i D^{R}_{BA}(\vec{x}t;\vec{x}t') = \theta(t-t') T_\Lambda \left\{ \frac{\rho}{2} \left[B_H(\vec{x},t), A_H(\vec{x}',t') \right] \right\}$$

↳ FUNÇÃO DE CORRELAÇÃO RETARDADA.

$$A_H(\vec{x},t) = e^{iHt} A(\vec{x}) e^{-iHt} = e^{iKt} A(\vec{x}) e^{-iKt}$$

SE $[A(\vec{x}), \hat{N}] = 0$

PARA UM CÁLCULO PERTURBATIVO, DEFINIMOS:

$$\mathcal{D}_{BA}(\vec{x},\tau;\vec{x}',\tau') = Tr\left\{\frac{\beta}{2} T_\tau\left[B_M(\vec{x},\tau) A_M(\vec{x}',\tau')\right]\right\}$$

ONDE:

$$B_M(\vec{x},\tau) = e^{K\tau} B(\vec{x}) e^{-K\tau}$$

$$A_M(\vec{x},\tau) = e^{K\tau} A(\vec{x}) e^{-K\tau}$$

QUE É PASSÍVEL DE UMA ABORDAGEM PERTURBATIVA PARA OBTERMOS D^R_{BA} A PARTIR DE $\mathcal{D}_{BA}$, USAMOS A REP. DE LEHMANN.

POR EXEMPLO, SE, COMO ANTES,

$$A(\vec{x}) = \tilde{m}(\vec{x}) = m(x) - m$$

$$B(\vec{x}) = A(x)$$

Representações de Lehmann

$$\Delta(\mathbf{q},\nu) = \frac{1}{Z}\sum_{m,n}\left\{e^{-\beta E_m}(2\pi)^4\,\delta\left[\nu-(E_n-E_m)\right]\delta^{(3)}\left[\mathbf{q}-(\mathbf{P}_n-\mathbf{P}_m)\right]\right.$$
$$\left.\left(1-e^{-\beta\omega}\right)\left|\langle m|\,\widetilde{n}\,(\mathbf{0})\,|n\rangle\right|^2\right\}$$

$$D^R_{\widetilde{n}\widetilde{n}}(\mathbf{q},\nu) = \int_{-\infty}^{+\infty}\frac{d\nu'}{2\pi}\frac{\Delta(\mathbf{q},\nu')}{\nu-\nu'+i\eta}$$

$$\mathcal{D}_{\widetilde{n}\widetilde{n}}(\mathbf{q},i\nu_n) = \int_{-\infty}^{+\infty}\frac{d\nu'}{2\pi}\frac{\Delta(\mathbf{q},\nu')}{i\nu_n-\nu'}$$

$$\widetilde{\Pi}(\vec{q},z)=\int_{-\infty}^{+\infty}\frac{d\nu'}{2\pi}\,\frac{\Delta(\vec{q},\nu')}{z-\nu'}$$

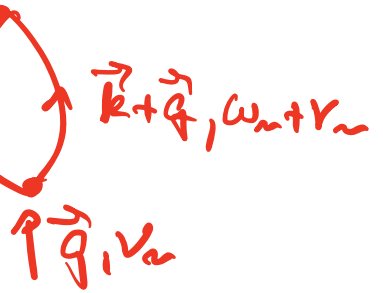
Note que nesse caso $i\nu_n$ é bosônica.

PARA O GÁS DE ELÉTRONS NO LIMITE DE ALTA DENSIDADE ($r_s \ll 1$), PODE-SE CALCULAR $D_{\tilde{n}\tilde{n}}$ EM RPA. DE MANEIRA GERAL:

$$D_{\tilde{n}\tilde{m}}(\vec{q}, \nu_n) = \tilde{\Pi}(\vec{q}, \nu_n) = \frac{\Pi(\vec{q}, \nu_n)}{1 - V(\vec{q})\Pi(\vec{q}, \nu_n)}$$

ASSIM COMO EM $T=0$, PARA $r_s \ll 1$:

$$\Pi(\vec{q}, \nu_n) \cong \Pi^{(0)}(\vec{q}, \nu_n) \Rightarrow$$



ν_n É BOSÔNICA

ω_n É FERMIÔNICA

$$\Rightarrow \Pi^{(0)}(\vec{q}, \nu_n) = 2T \sum_{\omega_n} \int \frac{d^3q}{(2\pi)^3} \frac{1}{i\omega_n - \epsilon_{\vec{k}}} \frac{1}{i\omega_n + i\nu_n - \epsilon_{\vec{k}+\vec{q}}}$$

$$G(x, y) = T \sum_{\omega_n} \frac{1}{(i\omega_n - x)(i\omega_n + i\nu_n - y)}$$

$$G(x,y) = \cancel{T} \int_C \frac{dz}{(2\pi i)} \frac{\cancel{-\beta}}{e^{\beta z}+1} \frac{1}{(z-x)(z+i\nu_n-y)}$$

$$= \int_{\Gamma \cup C'} \frac{dz}{2\pi i} \left(\quad \right)$$

↳ POLOS EM:

$z = x$

$z = y - i\nu_n$

A INTEGRAL SOBRE Γ É NOVAMENTE ZERO.

i) $\mathrm{Re}\, z > 0$: INTEGRANDO $\sim \dfrac{e^{-\beta R}}{R^2} \to 0$

ii) $\mathrm{Re}\, z < 0$: INTEGRANDO $\sim \dfrac{1}{R^2} R\,d\theta \to 0$

RESTA C':

$$G(x,y) = \left[\frac{1}{e^{\beta x}+1} \frac{1}{x-y+i\nu_n} + \frac{1}{e^{\beta y} \underbrace{e^{-i\nu_n \beta}}_{=1} + 1} \frac{-1}{x-y+i\nu_n} \right]$$

$$= \frac{f(x) - f(y)}{x-y+i\nu_n}$$

$$\Pi^{(0)}(\vec{q}, \nu_n) = -2 \int \frac{d^3k}{(2\pi)^3} \frac{f(\epsilon_{\vec{k}+\vec{q}}) - f(\epsilon_{\vec{k}})}{i\nu_n - [\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}]}$$

AGORA, PODEMOS FACILMENTE FAZER A CONT. ANALÍTICA:

$$\Pi^{(0)R}(\vec{q}, \nu) = -2 \int \frac{d^3k}{(2\pi)^3} \frac{f(\epsilon_{\vec{k}+\vec{q}}) - f(\epsilon_{\vec{k}})}{\nu + i\eta - [\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}]}$$

(i) CLARAMENTE, QUANDO $T \to 0$, RECUPERAMOS O RESULTADO A $T=0$.

(ii) É IMPORTANTE NOTAR QUE SÓ DEVEMOS FAZER $i\nu_n \longrightarrow \nu + i\eta$ APÓS A SOMA SOBRE FREQ. DE MATSUBARA. DO CONTRÁRIO TERÍAMOS

$$f(\epsilon_{\vec{k}+\vec{q}} - i\nu_n) \longrightarrow f(\epsilon_{\vec{k}+\vec{q}} - \nu - i\eta) \neq f(\epsilon_{\vec{k}+\vec{q}})$$