FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

2º Semestre de 2023
14/11/2023
Aula 25

Aulas passadas

Funções de Green de Matsubara: frequências de Matsubara

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

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

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

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

Funções de Green de Matsubara: caso não interagente

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

válida para férmions ou bósons.

Aula passada

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

$$\left(K_n = E_n - \mu N_n\right)$$

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

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

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

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

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

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

Aula passada

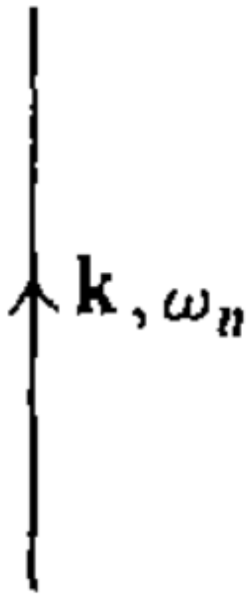
1. Draw all topologically distinct connected graphs with n interaction lines and $2n+1$ directed particle lines.
2. Assign a direction to each interaction line. Associate a wave vector and discrete frequency with each line and conserve each quantity at every vertex.
3. With each particle line associate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

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

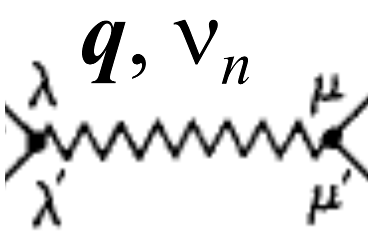
   where ω_m contains even (odd) integers for bosons (fermions).
4. Associate a factor $\mathscr{V}_0(\mathbf{k},\omega_m) \equiv V(\mathbf{k})$ with each interaction line.
5. Integrate over all n independent internal wave vectors and sum over all n independent internal frequencies.
6. The indices form 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



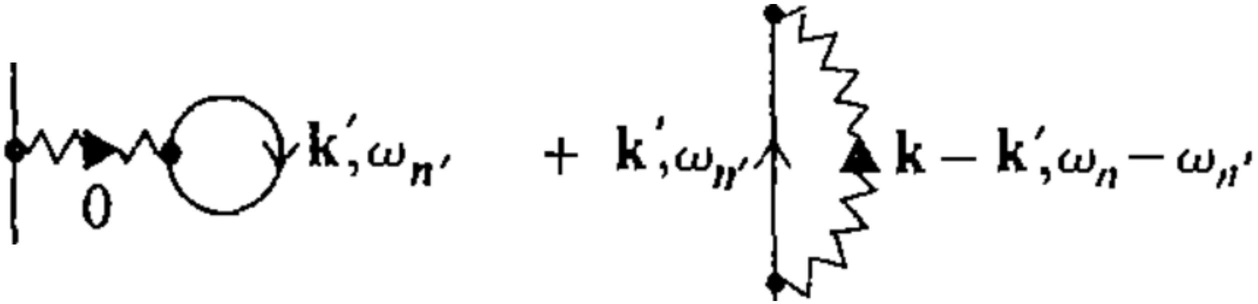
$$-\mathcal{G}^{(0)}_{\alpha\beta}\left(\mathbf{k}, i\omega_n\right) = -\frac{\delta_{\alpha,\beta}}{i\omega_n - \epsilon_{\mathbf{k}}}$$



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

Aula passada

Auto-energia em 1ª ordem:



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

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

Cálculo de somas de Matsubara

CONSIDERE A SEGUINTE FUNÇÃO:

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

$$\frac{\zeta\beta}{e^{\beta z} - \zeta} = \begin{cases} \dfrac{\beta}{e^{\beta z} - 1} & \text{(BÓSONS)} \\ \dfrac{-\beta}{e^{\beta z} + 1} & \text{(FÉRMIONS)} \end{cases}$$

(i) POLOS:

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

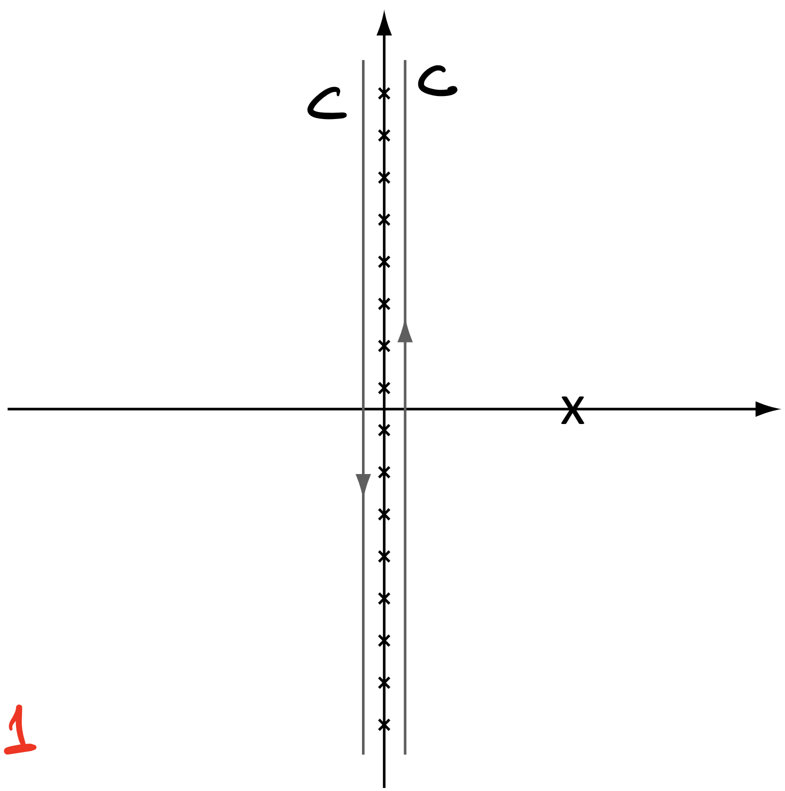
OU $\begin{cases} z_n = i\omega_n & (n \text{ par}) \\ z_n = i\omega_n & (n \text{ ímpar}) \end{cases}$

(ii) POLOS SIMPLES:

$$\frac{d}{dz}\left[e^{\beta z} - \zeta\right]\Big|_{z_n} = \beta e^{\beta z}\Big|_{z_n} = \beta\zeta$$

(iii) PRÓXIMO DOS POLOS:

$$\frac{\zeta\beta}{e^{\beta z} - \zeta} = \frac{\zeta\beta}{\zeta\beta(z - z_n)} = \frac{1}{z - z_n} \Rightarrow \text{RESÍDUO} = 1$$



ASSIM, PODEMOS ESCREVER:

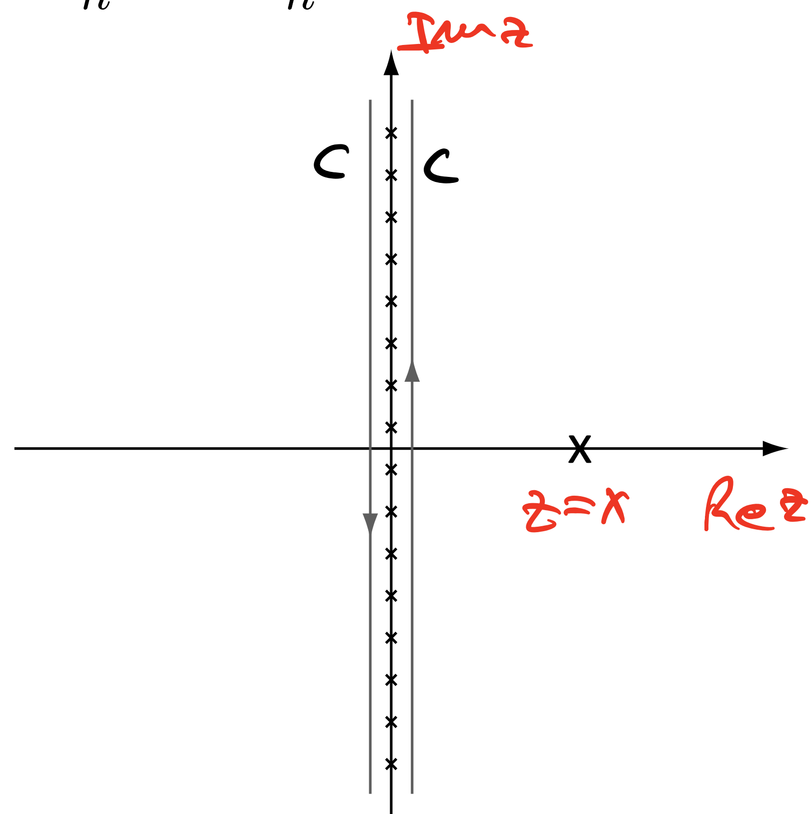
$$H(x) = \cancel{T} \int_C \frac{dz}{2\pi i} \frac{e^{\eta z}}{z-x} \left(\frac{\zeta \cancel{\beta}}{e^{\beta z} - \zeta} \right)$$

Cálculo de somas de Matsubara

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

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

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

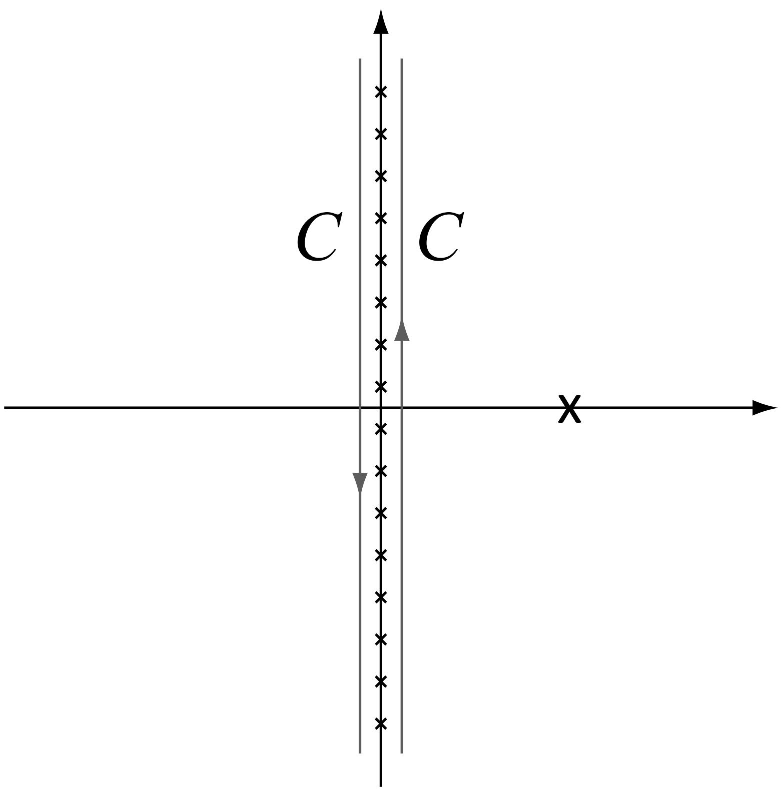


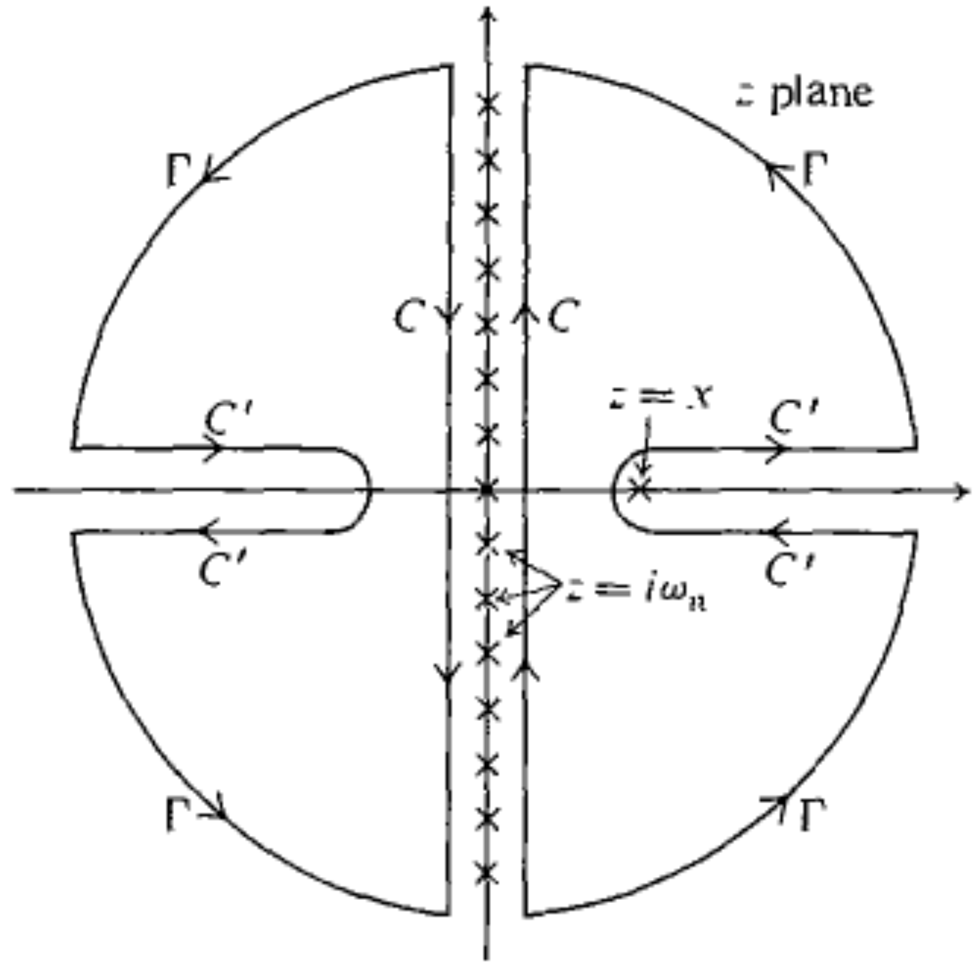
De maneira geral:

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

Cálculo de somas de Matsubara

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

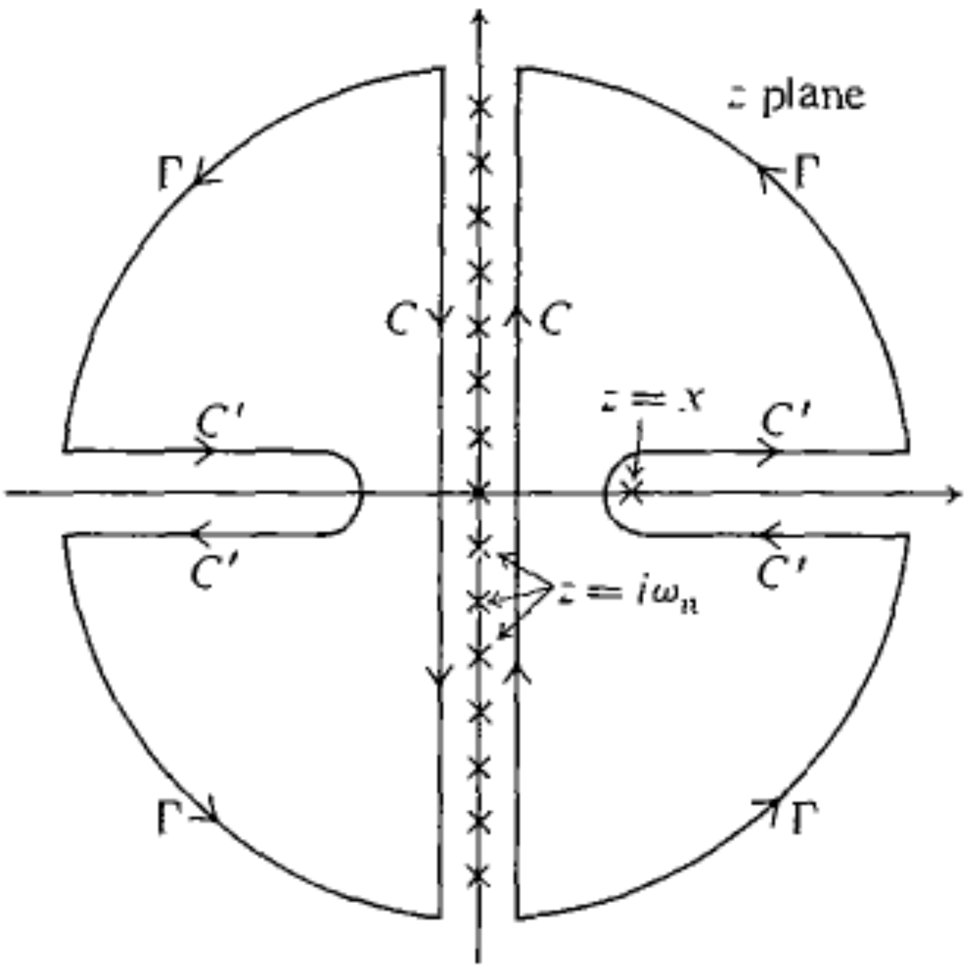




Deforma-se o caminho original C em G U C'

Cálculo de somas de Matsubara

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



A INTEGRAL EM Γ É ZERO:

(i) Re z > 0 : $|z| \to \infty$

INTEGRANDO: $\sim \dfrac{e^{(\eta-\beta)z}}{z} \to 0$

(ii) Re z < 0 : $|z| \to \infty$

INTEGRANDO: $\sim \dfrac{e^{\eta z}}{z} \to 0$

SOBRA APENAS O CAMINHO EM TORNO DE $z = x$ NO SENTIDO HORÁRIO

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

$$= -\zeta \frac{e^{\eta x}}{e^{\beta x} - \zeta} \xrightarrow[\eta \to 0]{} - \frac{\zeta}{e^{\beta x} - \zeta} = -\zeta f_\zeta(x)$$

ONDE:

$$f_\zeta(x) = \begin{cases} \dfrac{1}{e^{\beta x} - 1} & \text{(BÓSONS)} \\ \dfrac{1}{e^{\beta x} + 1} & \text{(FÉRMIONS)} \end{cases}$$

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

NOTE:

$$\int \frac{d^3 q}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_{\vec{q}} - \mu)} - \zeta} \neq \left\langle \frac{N}{V} \right\rangle$$

PORQUE $\mu \neq \mu_0$ = CASO NÃO INTERAGENTE

$$-\mathcal{G}^{(0)}(\vec{x},\tau) = \mathrm{Tr}\left[\frac{\rho}{Z} T_\tau[\psi(\vec{x},\tau)\psi^\dagger(0,0)]\right]$$

$\tau \to 0^-$:

$$\mathcal{G}^{(0)}(\vec{x},0^-) = -\zeta\, \mathrm{Tr}\left[\frac{\rho}{Z}\psi^\dagger(\vec{x})\psi(\vec{x})\right] = -\zeta \langle n(\vec{x})\rangle$$

ANALOGAMENTE, PODEMOS OBTER DE $\mathcal{G}^{(0)}(\vec{x},\tau)$ QUALQUER VALOR MÉDIO TÉRMICO DE OPERADORES DE UM CORPO.

E TAMBÉM, DE ALGUNS OPERADORES DE DOIS CORPOS, EM TOTAL ANALOGIA COM T=0.

ENTRETANTO, COISAS COMO A FUNÇÃO ESPECTRAL, EXIGEM O CÁLCULO DE G, G^R OU G^A:

$$A(\omega,\vec{k}) = \frac{1}{\pi}\,\mathrm{Im}\left[G^A(\omega,\vec{k})\right]$$

Resposta linear a temperatura finita

COMO VIMOS NO DESENVOLVIMENTO DA TEORIA DE RESPOSTA LINEAR EM T=0:

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

ONDE $H_{ext}(t)$ COMEÇA A ATUAR EM $t=t_0$. EM PARTICULAR ELEMENTOS DIAGONAIS GENÉRICOS SÃO:

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

TOMANDO O TRAÇO COM O PESO DE BOLTZMANN:

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

ONDE O TRAÇO É NO ENSEMBLE GRANDE CANÔNICO.

SE: $H_{ext}(t) = \int d^3x \; A(\bar{x})\,\phi(\vec{x},t)$ $\qquad \phi(\bar{x},t) \neq 0$ APENAS SE $t > t_0$

$$\Rightarrow \delta\langle \vec{B}(\bar{x},t)\rangle = -i\int_{t_0}^{t} dt' \int d^3x' \; \mathrm{Tr}\left\{\frac{\rho}{Z}\left[B_H(\bar{x},t), A_H(\bar{x}',t')\right]\right\}\phi(x',t')$$

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

ONDE:

$$i\,D^R_{BA}(x,x') \equiv \mathrm{Tr}\left\{\frac{\rho}{Z}\left[B_H(x), A_H(x')\right]\right\}\theta(t-t')$$

FUNÇÃO DE CORRELAÇÃO BA RETARDADA

GERALMENTE, A E B COMUTAM COM $\underline{N}$ E:

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

ONDE: $K = H - \mu N$

COMO EM T=0, A F.C. RETARDADA NÃO SE PRESTA FACILMENTE A UMA ABORDAGEM PERTURBATIVA. POR ISSO, DEFINIMOS SUA CONTRAPARTIDA DE MATSUBARA

$$-\mathcal{D}_{BA}(\bar{x},\tau;\bar{x}',\tau') = \mathrm{Tr}\left\{\frac{\rho}{Z} T_\tau\left[B_M(\bar{x},\tau)\, A_M(\bar{x}',\tau')\right]\right\}$$

ONDE: $A_M(\bar{x},\tau) = e^{K\tau} A(\bar{x})\, e^{-K\tau}$, ETC.

NO CASO ANALISADO ANTERIORMENTE DA DENSIDADE-DENSIDADE: $A(\bar{x}) = B(\bar{x}) = \tilde{n}(\bar{x}) = n(x) - n_0$

$$i\mathcal{D}^R_{\tilde{n}\tilde{n}}(x,x') = \theta(t-t')\,\mathrm{Tr}\left\{\frac{\rho}{Z}\left[\tilde{n}_H(\bar{x},t),\tilde{n}_H(\bar{x}',t')\right]\right\}$$

$$-\mathcal{D}_{\tilde{n}\tilde{n}}(\bar{x}\tau,\bar{x}',\tau') = \mathrm{Tr}\left\{\frac{\rho}{Z} T_\tau\left[\tilde{n}_M(\bar{x},\tau)\,\tilde{n}_M(\bar{x}',\tau')\right]\right\}$$

Representações de Lehmann

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

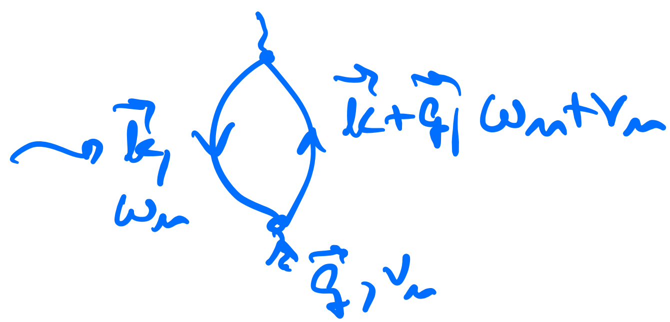
$$D^R_{\widetilde{n}\widetilde{n}}(\mathbf{q},\nu) = \int_{-\infty}^{+\infty}\frac{d\nu'}{2\pi}\frac{\Delta(\mathbf{q},\nu')}{\nu-\nu'+i\eta}$$
$$\mathcal{D}_{\widetilde{n}\widetilde{n}}(\mathbf{q},i\nu_n) = \int_{-\infty}^{+\infty}\frac{d\nu'}{2\pi}\frac{\Delta(\mathbf{q},\nu')}{i\nu_n-\nu'}$$

ESSA FREQUÊNCIA É BOSÔNICA

APLICANDO NO CASO DO GÁS DE ELÉTRONS DE ALTA DENSIDADE ($r_s \ll 1$). COMO A ESTRUTURA DOS DIAGRAMAS É A MESMA QUE A $T=0$:

$$D_{\hat{n}\hat{n}}(\vec{q},\nu_n) = \underbrace{\tilde{\Pi}(\vec{q},\nu_n)}_{\text{INS. POL. IMPRÓPRIA}} = \frac{\Pi(\vec{q},\nu_n)}{1 - V(\vec{q})\underbrace{\Pi(\vec{q},\nu_n)}_{\text{INS. POL. PRÓPRIA}}} \qquad V(\vec{q}) = \frac{4\pi e^2}{q^2}$$

$$-\Pi(\vec{q},\nu_n) \overset{r_s \ll 1}{\cong} -\Pi^{(0)}(\vec{q},\nu_n) \rightsquigarrow$$



ν_n: BOSÔNICA

ω_n: FERMIÔNICA

$$\cancel{-}\Pi^{(0)}(\vec{q},\nu_m) = \cancel{-}2T\sum_{\omega_m}\int\frac{d^3k}{(2\pi)^3}\,\mathcal{G}^{(0)}(\vec{k},\omega_m)\,\mathcal{G}^{(0)}(\vec{k}+\vec{q},\omega_m+\nu_m)$$

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

ONDE: $\epsilon_{\vec{k}} = \frac{k^2}{2m}-\mu = \frac{k^2}{2m}-\frac{k_F^2}{2m}$ $\quad x=\epsilon_{\vec{k}}$; $y=\epsilon_{\vec{k}+\vec{q}}$

$$T\sum_{\omega_m}\frac{1}{i\omega_m-x}\,\frac{1}{i\omega_m+i\nu_m-y} = \int_C\frac{dz}{2\pi i}\,\frac{-1}{e^{\beta z}+1}\left[\frac{1}{(z-x)(z+i\nu_m-y)}\right]$$

$[\ ]\to$ POLOS EM $z=x$ E $z=y-i\nu_m$

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

$$e^{\beta(y-i\nu_m)} = e^{\beta y}\,e^{-i\beta\nu_m} = e^{\beta y}$$

$$= \frac{1}{x - y + i\nu_m}\left[f(x) - f(y) \right]$$

ONDE: $f(x) = \frac{1}{e^{\beta x} + 1}$

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

PARA OBTER $D^R_{\hat{n}\hat{n}}(\vec{q}, \nu)$ FAZEMOS $i\nu_m \to \nu + i\eta$

$$D^R_{\hat{n}\hat{n}}(\vec{q}, \nu) = \frac{\Pi^{(0)R}(\vec{q}, \nu)}{1 - V(\vec{q})\, \Pi^{(0)R}(\vec{q}, \nu)}$$

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

ESSA É A FUNÇÃO DE LINDHARD A $T \neq 0$.

COMENTÁRIOS:

(i) SE $T \to 0$ $f(x) \to \theta(-x)$ E RECUPERAMOS O RESULTADO EM $T=0$.

(ii) É ERRADO FAZER $i\nu_n \to \nu + i\eta$ ANTES DE REALIZAR A SOMA SOBRE ω_n. SE TIVÉSSEMOS FEITO ISSO, TERÍAMOS:

$$\frac{1}{e^{\beta(y - i\nu_n)} + 1} \xrightarrow[i\nu_n \to \nu + i\eta]{} \frac{1}{e^{\beta(y-\nu)} + 1}$$

QUE É COMPLETAMENTE ERRADO. FAÇAM A SOMA DE MATSUBARA PRIMEIRAMENTE ATÉ O FIM E SÓ ENTÃO A CONT. ANALÍTICA: $i\nu_n \to \nu + i\eta$