Teoria de perturbação - T finita.

Refs.: Secs. 23 à 26, Fetter and Walecka.
Caps. 11 e 13, Bruus.
Sec. 30, Fetter and Walecka, } RPA
Cap. 14, Bruus,
Secs. 31 e 32, Fetter and Walecka.

ideia: introduzir a função de Green de tempo imaginário e sua determinação perturbativa via uma análise diagramática similar ao caso $T=0$;
considerar o gás de elétrons na random phase approximation (RPA) e
introduzir a função de Green a tempo real e determinar sua relação c/ a função de Green de tempo imaginário.

· sistemas a temperatura finita: nesse caso, é interessante utilizar o ensemble gran canônico;
considerar:

$$K = H - \mu N \qquad (242.1)$$

onde: $H$: hamiltoniano do sistema;
$N$: op. número total de partículas;
$\mu$: potencial químico.

↳ $Z = Tr\, e^{-\beta K} = Tr\, e^{-\beta(H-\mu N)} = e^{-\beta\Omega}$ : função de partição

$$\hat{\rho} = \frac{1}{Z} e^{-\beta K} = e^{\beta(\Omega - K)} \quad : \text{op. estatístico} \qquad (242.2)$$

onde $\beta = 1/k_B T$ e $\Omega = F - \mu N$: gran potencial termodinâmico

. nesse caso, é interessante introduzir operadores em uma versão de Heisenberg modificada;
p/ $H \neq H(t)$ e $O_S(\vec{r})$ : op. na versão de Schrödinger:

$$O_H(\vec{r},\tau) = e^{K\tau/\hbar}\, O_S(\vec{r})\, e^{-K\tau/\hbar} \qquad (243.1)$$

lembrar que, na rep. de Heisenberg usual:

$$O_H(\vec{r},t) = e^{iHt/\hbar}\, O_S(\vec{r})\, e^{-iHt/\hbar} \quad : \text{Eq. } (124.2)$$

notar: podemos considerar $\tau$ como imaginario puro e identificar:

$$\tau = it \qquad (243.2)$$

↳ Eqs. (124.2) e (243.1) : relacionadas via continuação analítica

. em particular, p/ ops. de campo:

$$\hat{\psi}_{H\alpha}(\vec{r},\tau) = e^{K\tau/\hbar}\, \hat{\psi}_{S\alpha}(\vec{r})\, e^{-K\tau/\hbar} \qquad (243.3)$$

⊕ notação: $\hat{\psi}_{H\alpha}(\vec{r},\tau) \to \psi_\alpha(\vec{r},\tau)$
$\hat{\psi}_{S\alpha}(\vec{r}) \to \psi_\alpha(\vec{r})$ ; $\alpha$ : índice spin

↳ $\psi_\alpha(\vec{r},\tau) = e^{K\tau/\hbar}\, \psi_\alpha(\vec{r})\, e^{-K\tau/\hbar}$
: (243.4)
e $\psi^+_\alpha(\vec{r},\tau) = e^{K\tau/\hbar}\, \psi^+_\alpha(\vec{r})\, e^{K\tau/\hbar}$

: comparar c/ Eq. (125.1)

notar: p/ $\tau \in \mathbb{R}$ → $\psi^+_\alpha(\vec{r},\tau) \neq \left(\psi_\alpha(\vec{r},\tau)\right)^+$

Obs.: introducção de tempo e frequência imaginários:
math trick, s/ significado físico;
útil p/ formulação teoria de perturbação.

· Definição: função de Green de tempo imaginário ou
" " " " Matsubara:

$$G_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau') = -\frac{1}{Z} \operatorname{Tr}\left[e^{-\beta K} T_\tau\left(\psi_\alpha(\vec{r},\tau)\,\psi^\dagger_\beta(\vec{r}',\tau')\right)\right] \qquad (244.1)$$

onde

$T_\tau$: op. ordenamento temporal p/ tempo imaginário,
similar op. (126.1) p/ tempo real;
em particular:

$$T_\tau\left(A(\tau)B(\tau')\right) = \theta(\tau-\tau')A(\tau)B(\tau') \pm \theta(\tau'-\tau)B(\tau')A(\tau) \; ;$$

sinal superior: bósons (244.2)
" inferior: férmions

e $\operatorname{Tr}(\ldots) = \sum_n \langle n|\ldots|n\rangle$
↳ base espaço de Hilbert.

· Definição: $\langle \hat{O} \rangle = \frac{1}{Z} \operatorname{Tr}\left(e^{-\beta K}\hat{O}\right)$ (244.3)

↳ Eq. (244.1) pode ser escrita como:

$$G_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau') = -\left\langle T_\tau\left[\psi_\alpha(\vec{r},\tau)\,;\,\psi^\dagger_\beta(\vec{r}',\tau')\right]\right\rangle : \qquad (244.4)$$

: notar similaridade c/ Eq. (127.1)

· propriedades da função de Green de Matsubara:

considerar: $C_{AB}(\tau,\tau') = -\langle T_\tau [A(\tau) B(\tau')] \rangle$ (245.1)

(i) $C_{AB}(\tau,\tau') = C_{AB}(\tau-\tau')$;

notar: p/ $\tau > \tau'$:

$$-C_{AB}(\tau,\tau') = \frac{1}{Z} Tr\left[ e^{-\beta K} \underbrace{T_\tau (A(\tau) B(\tau'))}_{A(\tau)B(\tau')} \right]$$

($\hbar = 1$)

prop. cíclica do Tr

$$\overbrace{e^{-\beta K} e^{K\tau} A_S e^{-K\tau} e^{K\tau'} B_S e^{-K\tau'}}$$

$$= \frac{1}{Z} Tr\left[ e^{-\beta K} e^{K(\tau-\tau')} A_S e^{-K(\tau-\tau')} B_S \right]$$

$$= \langle T_\tau [A(\tau-\tau') B(0)] \rangle$$

$$= -C_{AB}(\tau-\tau');$$

similar p/ $\tau' > \tau$.

(ii) possíveis valores $\tau$:

verifica-se que (veja pg. ): $0 \leq \tau \leq \beta\hbar$

$\hookrightarrow -\beta\hbar \leq \tau' \leq 0 \to -\beta\hbar \leq \tau-\tau' \leq \beta\hbar$ (245.2)

(iii) $C_{AB}(\tau) = \pm C_{AB}(\tau+\beta\hbar)$ ; $\tau < 0$ (245.3)

notar: ($\hbar = 1$) $-C_{AB}(\tau+\beta) = \frac{1}{Z} Tr\left[ e^{-\beta K} \underbrace{e^{K(\tau+\beta)} A_S e^{-K(\tau+\beta)}}_{e^{K\tau} A_S e^{-K\tau} e^{-\beta K}} B_S \right]$

(f) prop. cíclica do traço:

$$-C_{AB}(\tau+\beta) = \frac{1}{Z} \, Tr\left[ e^{-\beta K} \underbrace{B_S \, e^{K\tau} A_S \, e^{-K\tau}} \right]$$

$$B(0)\, A(\tau) = \pm T_\tau \big( A(\tau) B(0) \big)$$

$\tau < 0$

$$= \pm \underbrace{\frac{1}{Z} \, Tr\left[ e^{-\beta K} T_\tau \big( A(\tau) B(0) \big) \right]}$$

$$= -C_{AB}(\tau) \, ;$$

similar p/ $\tau > 0$.

· p/ função de Green (244.1):

(i) $\mathcal{G}_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau') = \mathcal{G}_{\alpha\beta}(\vec{r},\vec{r}',\tau-\tau')$

(246.1)

(iii) $\mathcal{G}_{\alpha\beta}(\vec{r},\vec{r}',\tau) = \pm \mathcal{G}_{\alpha\beta}(\vec{r},\vec{r}',\tau+\beta\hbar) \; ; \; \tau < 0$

· Como $\mathcal{G}_{\alpha\beta}(\vec{r},\vec{r}',\tau)$ é periódica/antiperiódica p/ $-\beta\hbar \leq \tau \leq \beta\hbar$

↳ " pode ser expandida em uma série de Fourier;

hipótese: $\mathcal{G}_{\alpha\beta}(\vec{r},\vec{r}',\tau) = \delta_{\alpha\beta} \, \mathcal{G}(\vec{r},\vec{r}',\tau)$;

temos que:

$$\mathcal{G}(\vec{r},\vec{r}',\tau) = \frac{1}{\beta\hbar} \sum_n e^{-i\omega_n \tau} \, \mathcal{G}(\vec{r},\vec{r}',\omega_n) \; ; \; \tau = \tau - \tau' \qquad (246.2)$$

onde $\omega_n = \dfrac{n\pi}{\beta\hbar}$ ; $n \in \mathbb{Z}$.

e $$\mathcal{G}(\vec{r},\vec{r}',\omega_n) = \frac{1}{2}\int_{-\beta\hbar}^{\beta\hbar} d\tau\, e^{-i\omega_n\tau}\, \mathcal{G}(\vec{r},\vec{r}',\tau) \tag{247.1}$$

· notar:

$$\mathcal{G}(\vec{r},\vec{r}',\tau+2\beta\hbar) = \frac{1}{\beta\hbar}\sum_n e^{-i\omega_n\tau}\, \exp\Big(\underbrace{-i\omega_n\cdot 2\beta\hbar}_{-i\frac{n\pi}{\beta\hbar}\cdot 2\beta\hbar = -2\pi n i}\Big)\, \mathcal{G}(\vec{r},\vec{r}',\omega_n)$$

$$= \mathcal{G}(\vec{r},\vec{r}',\tau) \tag{247.2}$$

· Eq. (247.1) pode ser escrita como:

$$\mathcal{G}(\vec{r},\vec{r}',\omega_n) = \underbrace{\frac{1}{2}\int_{-\beta\hbar}^{0} d\tau\, e^{-i\omega_n\tau}\, \underbrace{\mathcal{G}(\vec{r},\vec{r}',\tau)}_{\pm\mathcal{G}(\vec{r},\vec{r}',\tau+\beta\hbar)}}_{} + \frac{1}{2}\int_{0}^{\beta\hbar} d\tau\, e^{-i\omega_n\tau}\, \mathcal{G}(\vec{r},\vec{r}',\tau)$$

$\tau = \tau' - \beta\hbar$ :

$\tau' \to \tau$

$$\pm\int_0^{\beta\hbar} d\tau\, e^{-i\omega_n\beta\hbar}\, e^{-i\omega_n\tau}\, \mathcal{G}(\vec{r},\vec{r}',\tau)$$

$$= \frac{1}{2}\underbrace{\left(1 \pm e^{-i\omega_n\beta\hbar}\right)}_{1\pm e^{-in\pi} = 1\pm(-1)^n}\int_0^{\beta\hbar} d\tau\, e^{-i\omega_n\tau}\, \mathcal{G}(\vec{r},\vec{r}',\tau)$$

↳ p/ bósons: $\frac{1}{2}(1+(-1)^n) = \begin{cases} 1, & n \text{ par} \\ 0, & n \text{ impar} \end{cases}$ (247.3)

p/ férmions: $\frac{1}{2}(1-(-1)^n) = \begin{cases} 0, & n \text{ par} \\ 1, & n \text{ impar} \end{cases}$

$\hookrightarrow \mathcal{G}(\vec{r},\vec{r}\,',\omega_n) = \int_0^{\beta\hbar} d\tau \, e^{i\omega_n\tau} \mathcal{G}(\vec{r},\vec{r}\,',\tau)$,

onde: $\omega_n = \frac{2n\pi}{\beta\hbar}$ : bósons (248.1)

: frequências de Matsubara

$\omega_n = \frac{(2n+1)\pi}{\beta\hbar}$ : férmions

· p/ um sistema homogêneo (espaço), temos que

$$\mathcal{G}(\vec{r},\vec{r}\,',\tau) = \mathcal{G}(\vec{r}-\vec{r}\,',\tau) \;\; \text{e} \;\; \mathcal{G}(\vec{r},\vec{r}\,',\omega_n) = \mathcal{G}(\vec{r}-\vec{r}\,',\omega_n);$$

temos que:

$$\mathcal{G}_{\alpha\beta}(\vec{r}-\vec{r}\,',\tau) = \frac{1}{V}\sum_{\vec{k}} \frac{1}{\beta\hbar}\sum_n e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')} e^{-i\omega_n\tau} \mathcal{G}_{\alpha\beta}(\vec{k},\omega_n)$$

(248.2)

Veja pg. 47 $\curvearrowright$ $= \frac{1}{\beta\hbar}\sum_n \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')} e^{-i\omega_n\tau} \mathcal{G}_{\alpha\beta}(\vec{k},\omega_n)$

· próxima etapa: determinar relação entre
$\langle$observável$\rangle$ e $\mathcal{G}_{\alpha\beta}(\vec{r},\tau;\vec{r}\,',\tau')$;

notar:

$$\sum_\alpha \mathcal{G}_{\alpha\alpha}(\vec{r},\tau;\vec{r},\tau^+) = -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta K}\, \underbrace{T_\tau\left(\psi_\alpha(\vec{r},\tau)\,\psi^\dagger_\alpha(\vec{r},\tau^+)\right)}_{\pm\, \underbrace{\psi^\dagger_\alpha(\vec{r},\tau^+)\,\psi_\alpha(\vec{r},\tau)}_{e^{K\tau/\hbar}\psi^\dagger_\alpha(\vec{r})\underbrace{e^{-K\tau/\hbar}\,e^{K\tau/\hbar}}_{=1}\psi_\alpha(\vec{r})\,e^{-K\tau/\hbar}}}\right]$$

⊕ propriedade cíclica do traço:

$$\sum_\alpha G_{\alpha\alpha}(\vec{r},\tau;\vec{r},\tau^+) = \mp \frac{1}{Z} \mathrm{Tr}\Big[\underbrace{e^{-K\tau/\hbar}\, e^{-\beta K}\, e^{K\tau/\hbar}}_{e^{-\beta K}}\, \psi^\dagger_\alpha(\vec{r})\, \psi_\alpha(\vec{r})\Big]$$

$$= \mp \frac{1}{Z} \mathrm{Tr}\Big[e^{-\beta K}\, \psi^\dagger_\alpha(\vec{r})\, \psi_\alpha(\vec{r})\Big]$$

↳ $$\sum_\alpha G_{\alpha\alpha}(\vec{r},\tau;\vec{r},\tau^+) = \mp \langle \hat{n}(\vec{r}) \rangle \qquad (249.1)$$

↳ valor médio número (total) de partículas:

$$N = N(T,V,\mu) = \int d^3r\, \langle \hat{n}(\vec{r})\rangle = \mp \sum_\alpha \int d^3r\, G_{\alpha\alpha}(\vec{r},\tau;\vec{r},\tau^+) \qquad (249.2)$$

· similar p/ ops. 1 corpo/partícula:

como $\hat{O}(\vec{r}) = \sum_{\alpha\beta} \psi^\dagger_\beta(\vec{r})\, O_{\beta\alpha}(\vec{r})\, \psi_\alpha(\vec{r})$ : Eq. (128.3)

↳ $$\langle \hat{O}(\vec{r}) \rangle = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta K}\, \hat{O}(\vec{r})\right)$$

$$= \frac{1}{Z} \sum_{\alpha\beta} \mathrm{Tr}\left(e^{-\beta K}\, \psi^\dagger_\beta(\vec{r})\, O_{\beta\alpha}(\vec{r})\, \psi_\alpha(\vec{r})\right)$$

$$= \sum_{\alpha\beta} O_{\beta\alpha}(\vec{r})\, \underbrace{\frac{1}{Z} \mathrm{Tr}\left(e^{-\beta K}\, \psi^\dagger_\beta(\vec{r})\, \psi_\alpha(\vec{r})\right)}_{\lim_{\vec{r}'\to\vec{r}} \mp G_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau^+)}$$

(249.3)

↳ $$\langle \hat{O}(\vec{r}) \rangle = \mp \lim_{\vec{r}'\to\vec{r}} \sum_{\alpha\beta} O_{\beta\alpha}(\vec{r})\, G_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau^+)$$

Ex.: op. de energia cinética (36.3):

como $\hat{T} = \sum_\alpha \int d^3r\, \psi^\dagger_\alpha(\vec{r}) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \psi_\alpha(\vec{r})$

$$\hookrightarrow \langle \hat{T} \rangle = \mp \sum_\alpha \int d^3r \lim_{\vec{r}\,' \to \vec{r}} \left(-\frac{\hbar^2}{2m}\nabla^2\right) \mathcal{G}_{\alpha\alpha}(\vec{r},\tau;\vec{r}\,',\tau^+) : \qquad (250.1)$$

: comparar Eq. (130.2)

Ex.: termo de interação (37.1):

seguindo procedimento similar utilizado p/ determinar Eq. (131.1) [veja Eqs. (23.12) - (23.14), FetHen], verifica-se que:

$$\langle \hat{V} \rangle = \mp \frac{1}{2} \sum_\alpha \int d^3r \lim_{\vec{r}\,' \to \vec{r}} \left(-\hbar\frac{\partial}{\partial\tau} - \left(-\frac{\hbar^2}{2m}\nabla^2 - \mu\right)\right) \mathcal{G}_{\alpha\alpha}(\vec{r},\tau;\vec{r}\,',\tau^+)$$

(250.2)

$\hookrightarrow$ energia interna do sistema:

$$E = \langle \hat{T} + \hat{V} \rangle$$

$$= \mp \frac{1}{2} \sum_\alpha \int d^3r \lim_{\vec{r}\,' \to \vec{r}} \left(-\hbar\frac{\partial}{\partial\tau} - \frac{\hbar}{2m}\nabla^2 + \mu\right) \mathcal{G}_{\alpha\alpha}(r,\tau;\vec{r}\,',\tau^+)$$

(250.3)

Obs.: é possível expressar o potencial termodinâmico (242.2) $\Omega = \Omega(T,V,\mu)$ em termos de $\mathcal{G}^\lambda(\vec{r},\tau;\vec{r}\,',\tau^+)$; p/ detalhes, veja Eqs. (23.16) - (23.22), FetHen.

· em termos de $G_{\alpha\beta}(\vec{k},\omega_n)$, Eqs. (249.2) e (250.3) assumem a forma:

$$N = \mp \frac{1}{\beta\hbar} \sum_{\alpha} \sum_{n} \sum_{\vec{k}} e^{i\omega_n \eta} G_{\alpha\alpha}(\vec{k},\omega_n)$$

(251.1)

$$E = \langle \hat{T} + \hat{V} \rangle = \mp \frac{1}{2\beta\hbar} \sum_{\alpha} \sum_{n} \sum_{\vec{k}} e^{i\omega_n \eta} (i\hbar\omega_n + \epsilon^0_{\vec{k}} + \mu) G_{\alpha\alpha}(\vec{k},\omega_n)$$

notar: Eqs. (248.2) e (250.3):

$$E = \mp \frac{1}{2\beta\hbar} \cdot \frac{1}{V} \sum_{\alpha} \sum_{n} \sum_{k} \int d^3r \lim_{\tau' \to \tau^+} \lim_{\vec{r}' \to \vec{r}}$$

$$\underbrace{\left(-\hbar\partial_\tau - \frac{\hbar^2\nabla^2}{2m} + \mu\right) e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} e^{-i\omega_n(\tau-\tau')}}_{} G_{\alpha\alpha}(\vec{k},\omega_n)$$

$$\left(i\hbar\omega_n + \underbrace{\frac{\hbar^2 k^2}{2m}}_{\epsilon^0_{\vec{k}}} + \mu\right) e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} e^{-i\omega_n(\tau-\tau')}$$

$$= \mp \frac{1}{2\beta\hbar} \frac{1}{V} \sum_{\alpha} \sum_{n} \sum_{\vec{k}} \underbrace{\int d^3r}_{V} e^{i\omega_n \eta} (i\hbar\omega_n + \epsilon^0_{\vec{k}} + \mu) G_{\alpha\alpha}(\vec{k},\omega_n),$$

onde $\tau' - \tau = \eta$

Ex.: Função de Green de Matsubara p/ sistema não-interagente (bósons/férmions)

Lembrar hamiltoniano (132.4):

$$H_0 = \sum_\alpha \int d^3r\, \psi^\dagger_\alpha(\vec{r}) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \psi_\alpha(\vec{r}) = \sum_{\vec{k},\alpha} \epsilon_{\vec{k}}\, c^\dagger_{\vec{k}\alpha} c_{\vec{k}\alpha}$$

onde $\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$

$$\hookrightarrow K_0 = H_0 - \mu N = \sum_{\vec{k},\alpha} \underbrace{(\epsilon_{\vec{k}} - \mu)}_{\xi_{\vec{k}}} c^\dagger_{\vec{k}\alpha} c_{\vec{k}\alpha} \qquad (252.1)$$

Eq. (42.2): $\psi_\alpha(\vec{r}) = \frac{1}{V^{1/2}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} c_{\vec{k}\alpha}$

$$\hookrightarrow \psi_\alpha(\vec{r},\tau) = \frac{1}{V^{1/2}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \underbrace{e^{-\xi_k \tau/\hbar} c_{\vec{k}\alpha}}_{c_{\vec{k}\alpha}(\tau)\,:\ \text{veja pg. } 252.1}$$

(252.2)

$$\underline{\underline{e}}\ \psi^\dagger_\alpha(\vec{r},\tau) = \frac{1}{V^{1/2}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{r}} \underbrace{e^{\xi_k \tau/\hbar} c^\dagger_{\vec{k}\alpha}}_{c^\dagger_{\vec{k}\alpha}(\tau)}$$

Eq. (244.1):

$$-\mathcal{G}^0_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau') = \theta(\tau-\tau') \underbrace{\langle \psi_\alpha(\vec{r},\tau)\, \psi^\dagger_\beta(\vec{r}',\tau') \rangle}_{(\mathrm{I})} +$$

$$\pm\, \theta(\tau'-\tau) \underbrace{\langle \psi^\dagger_\beta(\vec{r}',\tau')\, \psi_\alpha(\vec{r},\tau) \rangle}_{(\mathrm{II})}$$

· sobre $C_{\vec{k}\alpha}(\tau)$ e $C^{\dagger}_{\vec{k}\alpha}(\tau)$:

como $C_{\vec{k}\alpha}(\tau) = e^{K\tau/\hbar}\, C_{\vec{k}\alpha}\, e^{-K\tau/\hbar}$

$\hookrightarrow\ \hbar\, \partial_\tau C_{\vec{k}\alpha}(\tau) = K e^{K\tau/\hbar} C_{\vec{k}\alpha} e^{-K\tau/\hbar} - e^{K\tau/\hbar} C_{\vec{k}\alpha} e^{-K\tau/\hbar} K$

$$= e^{K\tau/\hbar}\, \underbrace{[K, C_{\vec{k}\alpha}]}_{\sum_{p,\beta} \xi_p \underbrace{[C^{\dagger}_{p\beta} C_{p\beta} ; C_{\vec{k}\alpha}]}_{= -\delta_{\vec{p},\vec{k}}\, \delta_{\alpha\beta}\, C_{\vec{k}\alpha}}}\, e^{-K\tau/\hbar}$$

$\hookrightarrow\ \partial_\tau C_{\vec{k}\alpha}(\tau) = (-\xi_{\vec{k}}/\hbar)\, C_{\vec{k}\alpha}(\tau)$

$\hookrightarrow\ C_{\vec{k}\alpha}(\tau) = e^{-\xi_{\vec{k}}\tau/\hbar}\, C_{\vec{k}\alpha}(\tau = 0)$ ;

similar p/ $C^{\dagger}_{\vec{k}\alpha}(\tau)$.

notar:

$$(\mathrm{I}) = \frac{1}{V}\sum_{\vec{k},\vec{p}} e^{i\vec{k}\cdot\vec{r}-i\vec{p}\cdot\vec{r}'}\, e^{-\xi_{\vec{k}}\tau/\hbar+\xi_{\vec{p}}\tau'/\hbar}\, \underbrace{\langle C_{\vec{k}\alpha}C^{+}_{\vec{p}\beta}\rangle}_{\delta_{\vec{k},\vec{p}}\,\delta_{\alpha\beta}\,\pm\,\underbrace{\langle C^{+}_{\vec{p}\beta}C_{\vec{k}\alpha}\rangle}_{\frac{1}{Z}\underbrace{Tr\left(e^{-\beta\hat{K}}C^{+}_{\vec{p}\beta}C_{\vec{k}\alpha}\right)}_{\delta_{\alpha\beta}\,\delta_{\vec{k},\vec{p}}\,n_{\vec{k}}}}}$$

$$= \frac{1}{V}\delta_{\alpha\beta}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\, e^{-\xi_k(\tau-\tau')/\hbar}\,(1\pm n_{\vec{k}})$$

$$(\mathrm{II}) = \frac{1}{V}\sum_{\vec{k},\vec{p}} e^{i\vec{k}\cdot\vec{r}-i\vec{p}\cdot\vec{r}}\, e^{-\xi_{\vec{k}}\tau/\hbar+\xi_p\tau'/\hbar}\,\langle C^{+}_{\vec{p}\beta}C_{\vec{k}\alpha}\rangle$$

$$= \frac{1}{V}\delta_{\alpha\beta}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\, e^{-\xi_{\vec{k}}(\tau-\tau')/\hbar}\, n_{\vec{k}},$$

onde $n_{\vec{k}} = \dfrac{1}{e^{\beta\xi_{\vec{k}}}\mp 1}$ : $n_{BE}(\vec{k})$, $n_{FD}(\vec{k})$ (253.1)

$\hookrightarrow$ $$G^{0}_{\alpha\beta}(\vec{r}-\vec{r}',\tau-\tau') = -\frac{1}{V}\delta_{\alpha\beta}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\, e^{-\xi_{\vec{k}}(\tau-\tau')/\hbar}\, *$$

$$*\left(\Theta(\tau-\tau')(1\pm n_{\vec{k}})\pm\Theta(\tau'-\tau)\,n_{\vec{k}}\right) \quad : \qquad (253.2)$$

: comparar c/ Eq. (133.1)

· Eqs. (248.2) e (253.2)

$\hookrightarrow$ $$G^{0}_{\alpha\beta}(\vec{k},\tau) = -\delta_{\alpha\beta}\left(\Theta(\tau)(1\pm n_{\vec{k}})\pm\Theta(-\tau)\,n_{\vec{k}}\right)e^{-\xi_{\vec{k}}\tau/\hbar} \qquad (253.3)$$

· Eqs. (248.1) e (253.3):

· bósons:

$$\mathcal{G}^0_{\alpha\beta}(\vec{k},\nu_n) = \int_0^{\beta\hbar} d\tau \, e^{i\nu_n\tau}\, \mathcal{G}^0_{\alpha\beta}(\vec{k},\tau)$$

$$= -\delta_{\alpha\beta}\left(1 + n_{BE}(\vec{k})\right) \underbrace{\int_0^{\beta\hbar} d\tau \, \exp\left(\left(i\nu_n - \xi_k/\hbar\right)\tau\right)}_{\frac{1}{i\nu_n - \xi_{\vec{k}}/\hbar}\left(\underbrace{e^{i\nu_n\beta\hbar}}_{\exp\left(i\frac{2\pi n}{\beta\hbar}\beta\hbar\right)=1} e^{-\beta\xi_{\vec{k}}} - 1\right)}$$

$$= \underbrace{-\delta_{\alpha\beta}\underbrace{\left(1 + n_{BE}(\vec{k})\right)}_{\frac{e^{+\beta\xi_{\vec{k}}}}{e^{\beta\xi_{\vec{k}}}-1}}\left(e^{-\beta\xi_k} - 1\right)}_{=-1} \frac{1}{i\nu_n - \xi_{\vec{k}}/\hbar}$$

$$\hookrightarrow \mathcal{G}^0_{\alpha\beta}(\vec{k},\nu_n) = \frac{\delta_{\alpha\beta}}{i\nu_n - \xi_{\vec{k}}/\hbar} \quad ; \quad \nu_n = \frac{2n\pi}{\beta\hbar} \qquad (254.1)$$

· férmions:

$$\mathcal{G}^0_{\alpha\beta}(\vec{k},\omega_n) = -\delta_{\alpha\beta}\underbrace{\left(1 - n_{FD}(\vec{k})\right)}_{\frac{e^{\beta\xi_{\vec{k}}}}{e^{\beta\xi_{\vec{k}}}+1}} \underbrace{\int_0^{\beta\hbar} d\tau \, \exp\left(\left(i\omega_n - \xi_{\vec{k}}/\hbar\right)\tau\right)}_{\frac{1}{i\omega_n - \xi_{\vec{k}}/\hbar}(-1)\left(e^{-\beta\xi_{\vec{k}}}+1\right)}$$

$$\hookrightarrow \mathcal{G}^0_{\alpha\beta}(\vec{k},\omega_n) = \frac{\delta_{\alpha\beta}}{i\omega_n - \xi_{\vec{k}}/\hbar} \quad ; \quad \omega_n = \frac{(2n+1)\pi}{\beta\hbar} \qquad (254.2)$$

$$\xi_{\vec{k}} = \epsilon_{\vec{k}} - \mu$$

· notar: Eqs. (249.2) e (253.2):

$$N_0(T,V,\mu) = \mp \sum_\alpha \int d^3r \lim_{\tau'\to\tau^+} \lim_{\vec{r}'\to\vec{r}} G_{\alpha\alpha}(\vec{r}-\vec{r}';\underbrace{\tau-\tau'}_{-\eta<0})$$

$$= \mp \sum_\alpha \frac{(-1)}{V} (\pm) \sum_{\vec{k}} \underbrace{\int d^3r}_{V} \, n_{\vec{k}} \, e^{\xi_{\vec{k}}\eta/\hbar} = \sum_\alpha \sum_{\vec{k}} n_{\vec{k}} \qquad (255.1)$$

· similar, Eqs. (250.3) e (253.2):

$$E_0(T,V,\mu) = \mp \frac{1}{2} \sum_\alpha \int d^3r \lim_{\tau'\to\tau^+} \lim_{\vec{r}'\to\vec{r}} *$$

$$* \left(-\hbar\frac{\partial}{\partial\tau} - \frac{\hbar^2}{2m}\nabla^2 + \mu\right) G_{\alpha\alpha}(\vec{r}-\vec{r}';\tau-\tau')$$

$$= \mp \frac{1}{2} \sum_\alpha \frac{(-1)}{V} (\pm) \sum_{\vec{k}} \int d^3r \lim_{\tau'\to\tau^+} \lim_{\vec{r}'\to\vec{r}} *$$

$$* \underbrace{\left(-\hbar\partial_\tau - \frac{\hbar^2}{2m}\nabla^2 + \mu\right)}_{\xi_{\vec{k}} + \epsilon_{\vec{k}} + \mu \,=\, \epsilon_{\vec{k}} - \mu + \epsilon_{\vec{k}} + \mu \,=\, 2\epsilon_{\vec{k}}} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} e^{-\xi_{\vec{k}}(\tau-\tau')/\hbar} n_{\vec{k}}$$

$$= \sum_\alpha \sum_{\vec{k}} \epsilon_{\vec{k}} n_{\vec{k}} \qquad (255.2)$$

· próxima etapa: teoria de perturbação a temperatura finita.

inicial: versão/representação de interação (modificada):

considerar: $H(t) = H_0 + V(t) \rightarrow K(t) = \underbrace{H_0 - \mu N}_{} + V(t)$

notar hipótese $H_0 \neq H_0(t)$: $K_0 \neq K_0(t)$ (256.1)

similar Eq. (243.1), define-se:

$O_I(\tau) = e^{K_0\tau/\hbar}\, O_S\, e^{-K_0\tau/\hbar}$ : op. na versão de interação (256.2)

como $O_H(\tau) = e^{K\tau/\hbar}\, O_S\, e^{-K\tau/\hbar}$ ; Eq. (243.1) : op. na versão de Heisenberg

↳ $O_H(\tau) = \underbrace{e^{K\tau/\hbar}\, e^{-K_0\tau/\hbar}}_{=\tilde{U}(0,\tau)}\, \underbrace{e^{K_0\tau/\hbar}\, O_S\, e^{-K_0\tau/\hbar}}_{O_I(\tau)}\, \underbrace{e^{K_0\tau/\hbar}\, e^{-K\tau/\hbar}}_{=\tilde{U}(\tau,0)}$ (256.3)

de fato, é interessante definir o operador:

$\tilde{U}(\tau,\tau_0) = e^{K_0\tau/\hbar}\, e^{-K(\tau-\tau_0)/\hbar}\, e^{-K_0\tau_0/\hbar}$ : (256.4)

: comparar c/ Eq. (154.1)

· propriedades op. $\tilde{U}(\tau,\tau_0)$:

(1) $\tilde{U}^\dagger(\tau,\tau_0) \neq \tilde{U}(\tau_0,\tau)$ : NOT op. unitário;

(2) $\tilde{U}(\tau,\tau) = 1$ (256.5)

(3) $\tilde{U}(\tau_1,\tau_2)\tilde{U}(\tau_2,\tau_3) = \tilde{U}(\tau_1,\tau_3)$ : comparar c/ Eq. (154.3)

· equação de movimento:

$$\hbar \partial_\tau \tilde{U}(\tau,\tau_0) = K_0 \tilde{U}(\tau,\tau_0) - e^{K_0\tau/\hbar} K e^{-K(\tau-\tau_0)/\hbar} e^{-K_0\tau_0/\hbar}$$

$$= e^{K_0\tau/\hbar} \underbrace{(K_0 - K)}_{-V(t)} \underbrace{e^{-K(\tau-\tau_0)/\hbar}}_{} e^{-K_0\tau_0/\hbar} \quad e^{-K_0\tau/\hbar} \; e^{K_0\tau/\hbar}$$

$$= -V_I(\tau)\,\tilde{U}(\tau,\tau_0)$$

↳ $\hbar \dfrac{d}{d\tau} \tilde{U}(\tau,\tau_0) = -V_I(\tau)\,\tilde{U}(\tau,\tau_0)$ : eq. de movimento : p/ op. $\tilde{U}(\tau,\tau_0)$ :

⊕ c.i.: $\tilde{U}(\tau_0,\tau_0) = 1$ (257.1)

: comparar c/ Eq. (154.2)

· dada a similaridade entre Eqs. (154.2) e (257.1), temos que:

$$\tilde{U}(\tau,\tau_0) = \sum_{n\geq 0} \left(\frac{-1}{\hbar}\right)^n \frac{1}{n!} \int_{\tau_0}^{\tau} d\tau_1 \int_{\tau_0}^{\tau} d\tau_2 \ldots \int_{\tau_0}^{\tau} d\tau_n \, T_\tau\left[V_I(\tau_1)\ldots V_I(\tau_n)\right]$$

$$= T_\tau \exp\left(-\frac{1}{\hbar}\int_{\tau_0}^{\tau} d\tau' V_I(\tau')\right)$$ : expressão formal :

(257.2)

: comparar c/ Eq. (155.3)

· notar: $e^{-\beta K} = e^{-\beta K_0} e^{\beta K_0} e^{-\beta K} = e^{-\beta K_0}\,\tilde{U}(\beta\hbar, 0)$

⊕ Eqs. (242.2) e (257.2):

$$\hat{\rho} = \frac{1}{Z} e^{-\beta K} = \frac{1}{Z} e^{-\beta K_0}\, T_\tau \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau' V_I(\tau')\right) \qquad (257.3)$$

· Eqs. (256.3) e (257.3)

↳ expresson função de Green de Matsubara (244.1) em termos ops. de campo $\psi_{I\alpha}(\vec{r},\tau)$:

$$-\mathcal{G}_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau') = \frac{1}{Z}\,\mathrm{Tr}\Big[\underbrace{e^{-\beta K}\,T_\tau\big(\psi_{H\alpha}(\vec{r},\tau)\,\psi^{\dagger}_{H\beta}(\vec{r}',\tau')\big)}\Big]$$

$$e^{-\beta K_0}\,\tilde{U}(\beta\hbar,0)\,\underbrace{T_\tau\Big(\tilde{U}(0,\tau)\,\psi_{I\alpha}(\vec{r},\tau)\,\tilde{U}(\tau,\tau')\,\psi^{\dagger}_{I\beta}(\vec{r}',\tau')\,\tilde{U}(\tau',0)\Big)}$$

$$= T_\tau\Big(\underbrace{\tilde{U}(0,\tau)\,\tilde{U}(\tau,\tau')\,\tilde{U}(\tau',0)}_{\tilde{U}(0,0)=1}\,\psi_{I\alpha}(\vec{r},\tau)\,\psi^{\dagger}_{I\beta}(\vec{r}',\tau')\Big) \qquad (258.1)$$

devido propriedades op. $T_\tau$

como $Z = \mathrm{Tr}\, e^{-\beta K} = \mathrm{Tr}\big(e^{-\beta K_0}\,\tilde{U}(\beta\hbar,0)\big)$ : Eq. (242.2)

↑ Eq. (257.3)

$$\text{e} \quad Z_0 = \mathrm{Tr}\, e^{-\beta K_0} \qquad (258.2)$$

$$\hookrightarrow \; Z = Z_0\,\frac{1}{Z_0}\,\mathrm{Tr}\big(e^{-\beta K_0}\,\tilde{U}(\beta\hbar,0)\big) = \langle \tilde{U}(\beta\hbar,0)\rangle_0$$

$$\text{e} \quad \frac{1}{Z_0}\,\mathrm{Tr}\Big[e^{-\beta K_0}\,\tilde{U}(\beta\hbar,0)\,T_\tau\big(\psi_{I\alpha}(\vec{r},\tau)\,\psi^{\dagger}_{I\beta}(\vec{r}',\tau')\big)\Big] =$$

$$= \langle \tilde{U}(\beta\hbar,0)\,T_\tau\big(\psi_{I\alpha}(\vec{r},\tau)\,\psi^{\dagger}_{I\beta}(\vec{r}',\tau')\big)\rangle_0$$

$$\hookrightarrow \; \mathcal{G}_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau') = -\,\frac{\langle \tilde{U}(\beta\hbar,0)\,T_\tau\big(\psi_{I\alpha}(\vec{r},\tau)\,\psi^{\dagger}_{I\beta}(\vec{r}',\tau')\big)\rangle_0}{\langle \tilde{U}(\beta\hbar,0)\rangle_0} \qquad (258.3)$$

ou

$$G_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau') = -\frac{1}{Z}\,Tr\left[e^{-\beta K_0}\,\tilde{U}(\beta\hbar,0)\,T_\tau\left(\psi_{I\alpha}(\vec{r},\tau)\psi^\dagger_{I\beta}(\vec{r}',\tau')\right)\right]$$

$$\text{onde } Z = Tr\left(e^{-\beta K_0}\,\tilde{U}(\beta\hbar,0)\right) \tag{259.1}$$

· Eqs. (257.2) e (259.1):

$$G_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau') = -\frac{1}{Z}\,Tr\Big[e^{-\beta K_0}\sum_{n\geq 0}\left(\frac{-1}{\hbar}\right)^n\frac{1}{n!}\int_0^{\beta\hbar}d\tau_1\ldots d\tau_n \,*$$

$$*\; T_\tau\left(V_I(\tau_1)\ldots V_I(\tau_n)\,\psi_{I\alpha}(\vec{r},\tau)\,\psi^\dagger_{I\beta}(\vec{r}',\tau')\right)\Big]$$

onde

$$Z = Tr\left[e^{-\beta K_0}\sum_{n\geq 0}\left(\frac{-1}{\hbar}\right)^n\frac{1}{n!}\int_0^{\beta\hbar}d\tau_1\ldots d\tau_n\,T_\tau\left(V_I(\tau_1)\ldots V_I(\tau_n)\right)\right]: \tag{259.2}$$

: comparar c/ Eq. (161.1)

Obs.: similar formalismo $T=0$, o denominador $Z$ de (259.2)
↳ eliminação dos diagramas desconectados!

· sobre o teorema de Wick,

- similaridade entre Eqs. (161.1) e (259.2)
↳ série perturbativa $G$ similar
" " $\mathcal{G}$ !

- Matsubara: generalização teorema de Wick p/ $T\neq 0$.

· nesse caso: definição contração entre ops. A e B:

$$\overbrace{AB} = \langle T_\tau [AB] \rangle_0 = \frac{1}{Z_0} \operatorname{Tr} \left[ e^{-\beta K_0} T_\tau (AB) \right] : \qquad (260.1)$$

: comparar c/ Eq. (163.2):

: notar ausência ordem normal!

$$\hookrightarrow \overbrace{\psi_{I\alpha}(\vec{n},\tau)\,\psi^{+}_{I\beta}(\vec{n}',\tau')} = \frac{1}{Z_0} \operatorname{Tr} \left[ e^{-\beta K_0} \underbrace{T_\tau \left( \psi_{I\alpha}(\vec{n},\tau)\,\psi^{+}_{I\beta}(\vec{n}',\tau') \right)} \right]$$

veja Eq. (258.1) $\;\; = T_\tau \left( \psi_{H\alpha}(\vec{n},\tau)\,\psi^{+}_{H\beta}(\vec{n}',\tau') \right)$

$$= - G^{0}_{\alpha\beta}(\vec{n},\tau;\vec{n}',\tau') : \qquad (260.2)$$

: veja Eq. (167.3)

· teorema de Wick:

$$\langle T_\tau (AB \ldots F) \rangle_0 = \frac{1}{Z_0} \operatorname{Tr} \left[ T_\tau (AB \ldots F) \right] =$$

= soma todos os possíveis pares de contração : (260.3)

: comparar c/ Eq. (164.1)

Demonstração: veja pgs 237 - 241, Fetter;
" Sec. 11.6, Bruus

· próxima etapa: análise diagramática (259.2)!

· Análise diagramática,

novamente: similaridade série perturbativa $G(T=0)$

e " " $\mathcal{G}(T\neq 0)$;

notar:

$$\langle T_\tau [\, \psi_\alpha(1)\, \psi_\beta(2)\, \psi^\dagger_\mu(3)\, \psi^\dagger_\nu(4) \rangle_0 = (I),$$

onde $i = (\vec{r}_i, \tau_i)$, $i = 1,2,3,4$ e $\psi_\alpha(1) = \psi_{I\alpha}(\vec{r}_1, \tau_1)$;

⊕ teorema de Wick (260.3):

$$(I) = \pm\, \psi_\alpha(1)\, \psi^\dagger_\mu(3)\, \psi_\beta(2)\, \psi^\dagger_\nu(4) + \psi_\alpha(1)\, \psi^\dagger_\nu(4)\, \psi_\beta(2)\, \psi^\dagger_\mu(3)$$

$$= \pm\, \mathcal{G}^0_{\alpha\mu}(1,3)\, \mathcal{G}^0_{\beta\nu}(2,4) + \mathcal{G}^0_{\alpha\nu}(1,4)\, \mathcal{G}^0_{\beta\mu}(2,3) \qquad (261.1)$$

novamente:

numerador (259.2) = diagramas conectados

⊕ " desconectados

cancelamento via denominador $Z$ !

↳ Eq. (259.2):

$$\mathcal{G}_{\alpha\beta}(1,2) = -\sum_{n\geq 0} \left(\frac{-1}{\hbar}\right)^n \frac{1}{n!} \int_0^{\beta\hbar} d\tau'_1 \ldots d\tau'_n \,+$$

$$+ \frac{1}{Z_0} \mathrm{Tr}\left[ e^{-\beta K_0}\, T_\tau \left( V_I(\tau'_1) \ldots V_I(\tau'_n)\, \psi_\alpha(1)\, \psi^\dagger_\beta(2) \right) \right]_{\text{conectados}} :$$

(261.2)

: comparar c/ Eq. (174.2)

· considerar: potencial de interação entre duas partículas independente spin:

$$V = \frac{1}{2}\sum_{\alpha\beta}\int d^3r_1 d^3r_2\ \psi^+_\alpha(\vec{r}_1)\,\psi^+_\beta(\vec{r}_2)\,V(\vec{r}_1-\vec{r}_2)\,\psi_\beta(\vec{r}_2)\,\psi_\alpha(\vec{r}_1) :$$

: Eq. (43.3);

similar Eq. (162.2), verifica-se que, na representação de interação:

$$V_I(\tau_1) = \frac{1}{2}\sum_{\alpha\beta}\int d^3r_1 d^3r_2 \int_0^{\beta\hbar} d\tau_2\ +$$

$$+\ \psi^+_\alpha(\vec{r}_1,\tau_1)\,\psi^+_\beta(\vec{r}_2,\tau_2)\,V(\vec{r}_1-\vec{r}_2)\,\delta(\tau_1-\tau_2)\,\psi_\beta(\vec{r}_2,\tau_2)\,\psi_\alpha(\vec{r}_1,\tau_1),$$

onde $\psi_\alpha(1) = \psi_{I\alpha}(1)$ : índice I : omitido

(262.1)

e $U(\vec{r}_1,\tau_1;\vec{r}_2,\tau_2) = U(1,2) = V(\vec{r}_1-\vec{r}_2)\,\delta(\tau_1-\tau_2)$

· próxima etapa: reescrever regras p/ determinação diagramas de Feynman caso $T=0$ (pg. 175) p/ caso $T\neq 0$ !

· Regras p/ determinação diagramas de Feynman de ordem $\underline{\underline{n}}$ no espaço de coordenadas - $T \neq 0$:

(1) desenhar todos os diagramas conectados e topologicamente distintos c/ n linhas de interação - - - - -
e " $2n+1$ propagadores livres $\longleftarrow$ ;

(2) associar ao pto inicial as variáveis $2, \beta = \vec{r}_2, \tau_2, \beta$,
" " " final " " $1, \alpha = \vec{r}_1, \tau_1, \alpha$
e " aos $2n$ vértices (internos) " " $(3, \mu)$ ; $(4, \nu)$ ; ... ;

(3) cada linha contínua $\underset{1}{\overset{\alpha}{\phantom{x}}}\longleftarrow\underset{2}{\overset{\beta}{\phantom{x}}}$ corresponde a $\mathcal{G}^0_{\alpha\beta}(1,2)$;

(4) cada linha tracejada $\underset{1}{}$ - - - - - $\underset{2}{}$ corresponde ao

potencial $U(1,2)$ : veja Eq. (262.1)

(5) integrar sob índices internos $3, 4, \ldots$, i.e.,

$$\int d^3 r_i \int_0^{\beta\hbar} d\tau_i \quad ; \quad i = 3, 4, \ldots$$

e somar sob índices internos $\mu, \nu, \ldots$ ;

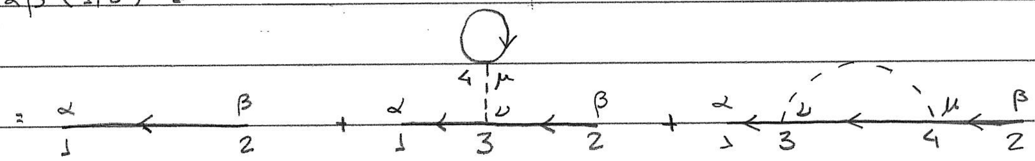
(6) multiplicar pelo fator $(-1)^F (-1/\hbar)^n$,
onde $F$ : # loops fermiônicos fechados e

(7) funções de Green c/ variáveis temporais iguais devem ser interpretadas como:

$$\mathcal{G}^0_{\alpha\beta}(\vec{r}, \tau ; \vec{r}', \tau^+) \qquad (263.1)$$

Ex. 1: diagramas ordem zero e 1ª ordem, veja Eq. (171.1):

$$G_{\alpha\beta}(1,2) =$$



⊕ Eq. (263.1):

$$G_{\alpha\beta}(1,2) = G^0_{\alpha\beta}(1,2)$$

$$\pm \frac{(-1)}{\hbar} \sum_{\mu\nu} \int d^3r_3\, d^3r_4 \int_0^{\beta\hbar} d\tau_3\, d\tau_4\; G^0_{\alpha\nu}(1,3)\, G^0_{\nu\beta}(3,2)\, G^0_{\mu\mu}(4,4)\, U(3,4)$$

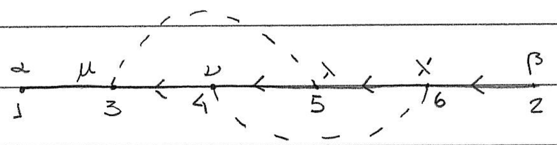
$(-1)^F = 1$

$$+ \frac{(-1)}{\hbar} \sum_{\mu\nu} \int d^3r_3\, d^3r_4 \int_0^{\beta\hbar} d\tau_3\, d\tau_4\; G^0_{\alpha\nu}(1,3)\, G^0_{\nu\mu}(3,4)\, G^0_{\mu\beta}(4,2)\, U(3,4)$$

(264.1)

Ex. 2: diagrama de 2ª ordem:

considerar o diagrama (2), Eq. (176.1):



$$\hookrightarrow\; G^{(2)}_{\alpha\beta}(1,2) = \underset{(-1)^F=0}{+} \left(\frac{-1}{\hbar}\right)^2 \sum_{\mu\nu\lambda\lambda'} \int d^3r_3\, d^3r_4\, d^3r_5\, d^3r_6 \int_0^{\beta\hbar} d\tau_3\, d\tau_4\, d\tau_5\, d\tau_6\, \times$$

$$\times\; G^0_{\alpha\mu}(1,3)\, G^0_{\mu\nu}(3,4)\, G^0_{\nu\lambda}(4,5)\, G^0_{\lambda\lambda'}(5,6)\, G^0_{\lambda'\beta}(6,2)\, \times$$

$$\times\; U(3,5)\, U(5,6)$$

(264.2)

· Diagramas de Feynman no espaço de momentos.

transformada de Fourier potencial (262.1):

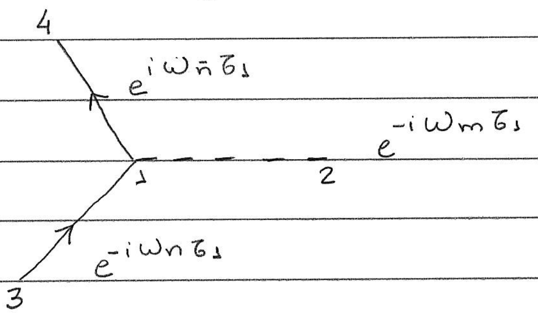
$$U(1,2) = \frac{1}{\beta\hbar} \sum_{n\ par} e^{-i\omega_n(\tau_1-\tau_2)}\, U(\vec{r}_1, \vec{r}_2, \omega_n) \qquad (265.1)$$

em particular, p/ $V(\vec{r}_1,\vec{r}_2) = V(\vec{r}_1-\vec{r}_2)$, temos que

$$U(1,2) = \frac{1}{V}\sum_{\vec{k}} \frac{1}{\beta\hbar}\sum_{n\ par} e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}\, e^{-i\omega_n(\tau_1-\tau_2)}\, U(\vec{k},\omega_n) \qquad (265.2)$$

notar: veja comentário abaixo!

similar Eq. (179.4), vamos considerar um vértice interno de um diagrama arbitrário de ordem $\underline{n}$:




(265.3)

notar: 1 - - - - 2 : $U(1,2) \sim e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}\, e^{-i\omega_m(\tau_1-\tau_2)}$

1 ←—— 3 : $G^0(1,3) \sim e^{i\vec{q}\cdot(\vec{r}_1-\vec{r}_3)}\, e^{-i\omega_n(\tau_1-\tau_3)}$

4 ←—— 1 : $G^0(4,1) \sim e^{i\vec{p}\cdot(\vec{r}_4-\vec{r}_1)}\, e^{-i\omega_{\bar{n}}(\tau_4-\tau_1)}$

como 1: pto interno diagrama, há uma integração sob $\vec{r}_1$ e $\tau_1$; em particular, p/ a integral temporal, temos que:

$$\int_0^{\beta\hbar} d\tau_1 \, \exp\left(-i(\omega_n - \omega_{\bar{n}} + \omega_m)\tau_1\right) =$$

$= \beta\hbar \, \delta_{\omega_n+\omega_m,\omega_{\bar{n}}}$ : conservação frequências discretas em cada vértice! (266.1)

notar: $\underbrace{\omega_{\bar{n}} - \omega_n}_{\text{pares ou ímpares}} = \omega_m$

pares ou ímpares e par : combinação OK!

Obs.: lembrar identidade:

$$\delta(\tau) = \frac{1}{\beta\hbar} \sum_{n \text{ par}} e^{-i\omega_n\tau} \quad ; \quad -\beta\hbar \leq \tau \leq \beta\hbar \qquad (266.2)$$

$$\text{e} \quad \delta_{\omega_n,0} = \frac{1}{\beta\hbar}\int_0^{\beta\hbar} d\tau \, e^{i\omega_n\tau}$$

· próxima etapa: reescrever regras (181.1) p/ determinação diagramas de Feynman caso $T=0$ p/ caso $T \neq 0$;

novamente: considerar sistema espacialmente homogêneo, i.e.,

$$G(\vec{r}_1, \vec{r}_2, \tau_1 - \tau_2) = G(\vec{r}_1 - \vec{r}_2, \tau_1 - \tau_2)$$

· Regras p/ determinação diagramas de Feynman de ordem $\underline{\underline{n}}$ no espaço de momentos - $T \neq 0$:

(1) desenhar todos os diagramas conectados e topologicamente distintos c/ n linhas de interação - - ← - -

$\underline{\underline{e}}$ " $2n+1$ " " partículas ——←——;

(2) associar um sentido a cada linha,

" " momento e frequência discreta a cada linha de partícula $\underline{\underline{e}}$

" " momento e frequência discreta para a cada linha de interação;

observar a conservação de momento e frequência discreta em cada vértice;

(3) cada linha contínua $\underset{\alpha \qquad\quad \beta}{\xleftarrow{\vec{k},\, \omega_n}}$ corresponde à

função de Green (254.1)/(254.2) $G^0_{\alpha\beta}(\vec{k}, \omega_n) = \delta_{\alpha\beta}\, G^0(\vec{k}, \omega_n)$;

(4) cada linha tracejada $\xleftarrow{\vec{q},\, \nu_n}$ corresponde ao potencial (265.2) $U(\vec{q}, \nu_n) = V(\vec{q})$;

(5) integrar sob os momentos (internos) $q_1, q_2, \ldots, q_n$,

somar " " frequências (internas) $\omega_{n1}, \omega_{n2}, \ldots \omega_{nn}$ $\underline{\underline{e}}$

" " indices internos $\mu, \nu, \ldots$;

(6) multiplicar pelo fator $(-1)^F \left( \dfrac{-1}{\beta \hbar^2 (2\pi)^3} \right)^n$,

notar limite $V \to +\infty$

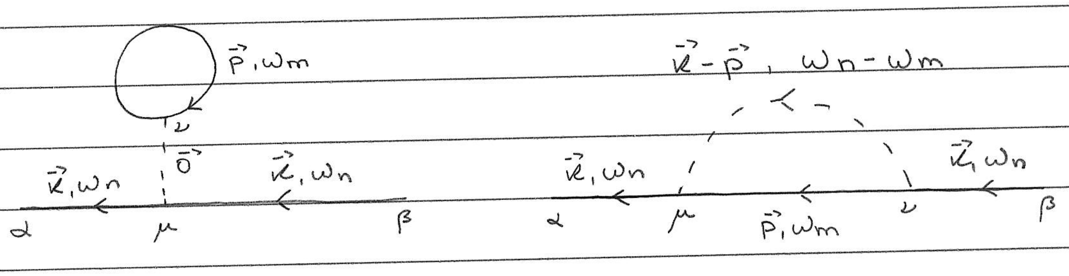
onde $F$: # loops fermiônicos fechados e

$\underline{\underline{e}}$

(7) p/ linhas de partículas associadas a índices temporais iguais (loops ou aqueles c/ pts inicial e final conectados por uma linha de interação) multiplicar pelo fator $e^{i\omega_n \eta}$, $\eta \to 0^+$.

(268.1)

Ex.: diagramas de 1ª ordem, veja Eq. (182.1):




⊕ regras (268.1):

$$G^{(1)}_{\alpha\beta}(\vec{k}, \omega_n) =$$

$$= \frac{+}{(-1)^F} \left(\frac{-1}{\beta\hbar^2}\right) \sum_{\mu\nu} \sum_m \int \frac{d^3p}{(2\pi)^3} \, U(0) \, G^0_{\alpha\mu}(\vec{k}, \omega_n) \, G^0_{\nu\nu}(\vec{p}, \omega_m) \, G^0_{\mu\beta}(\vec{k}, \omega_n) \, * \, e^{i\omega_m \eta}$$

$$+ \left(\frac{-1}{\beta\hbar^2}\right) \sum_{\mu\nu} \sum_m \int \frac{d^3p}{(2\pi)^3} \, U(\vec{k}-\vec{p}) \, G^0_{\alpha\mu}(\vec{k}, \omega_n) \, G^0_{\mu\nu}(\vec{p}, \omega_m) \, G^0_{\nu\beta}(\vec{k}, \omega_n) \, * \, e^{i\omega_m \eta},$$

como $G^0_{\alpha\beta}(\vec{k}, \omega_n) = \delta_{\alpha\beta} G^0(\vec{k}, \omega_n)$ e $\sum_\nu 1 = 2S+1$, temos que

$$G^{(1)}_{\alpha\beta}(k, \omega_n) = \delta_{\alpha\beta} \left( G^0(k, \omega_n) \right)^2 \left(\frac{-1}{\beta\hbar^2}\right) \sum_m \int \frac{d^3p}{(2\pi)^3} \, e^{i\omega_m \eta} \, *$$

$$* \left( \pm(2S+1) V(0) + V(\vec{k}-\vec{p}) \right) G^0(\vec{p}, \omega_m) \qquad (268.2)$$

· incluindo a contribuição de ordem zero, verifica-se que $G_{\alpha\beta}(\vec{k},\omega_n) = \delta_{\alpha\beta}\, G(\vec{k},\omega_n)$ apresenta a estrutura:

$$G(\vec{k},\omega_n) = G^0(\vec{k},\omega_n) + G^0(\vec{k},\omega_n)\,\Sigma(\vec{k},\omega_n)\,G^0(\vec{k},\omega_n), \tag{269.1}$$

similar Eq. (183.2);

em particular, autoenergia em 1ª ordem:

$\hbar\,\Sigma^{(1)}(\vec{k},\omega_n) = \hbar\,\Sigma(\vec{k}) =$

$$= -\frac{1}{\beta\hbar}\sum_m \int \frac{d^3p}{(2\pi)^3}\, e^{i\omega_m \eta}\left(\pm(2S+1)V(0) + V(\vec{k}-\vec{p})\right) \underbrace{G^0(\vec{p},\omega_m)}_{\overset{\text{Eq. (254.1)/(254.2)}}{=} \frac{1}{i\omega_m - \varepsilon_{\vec{p}}/\hbar}} \tag{269.2}$$

notar Eq. (269.2) : determinação $\Sigma(\vec{k}) \sim$ determinação soma sob frequências de Matsubara!

· sobre o cálculo da soma sob frequências de Matsubara:
(p/ detalhes, veja Sec. 25, Fetter e Sec. 11.4, Bruus);
como exemplificado em (269.2), é necessário determinar:

$$I_B = \frac{1}{\beta\hbar}\sum_n g(i\nu_n)\, e^{i\nu_n \eta} \quad ; \quad \nu_n = 2n\pi/\beta\hbar \ : \text{bósons}, \quad \eta > 0 \tag{269.2}$$

$$I_F = \frac{1}{\beta\hbar}\sum_n g(i\omega_n)\, e^{i\omega_n \eta} \quad ; \quad \omega_n = (2n+1)\pi/\beta\hbar \ : \text{férmions}$$

(1) bósons:

notar:

$$n_{BE}(z) = \frac{1}{e^{\beta\hbar z} - 1} \quad : \quad \text{polos}: \; \beta\hbar z = 2n\pi i$$

$$\hookrightarrow z = 2n\pi i/\beta\hbar = i\nu_n$$

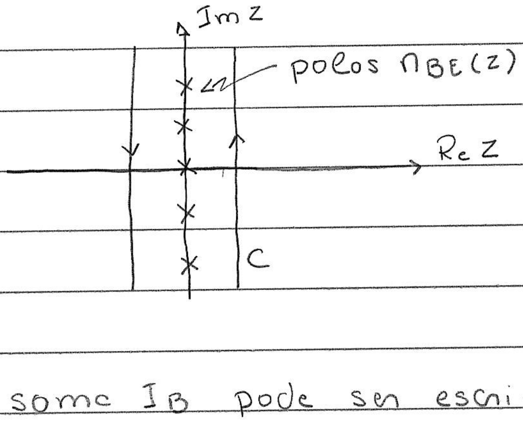
e

$$\underset{z=i\nu_n}{\text{Res}} \left( n_{BE}(z) \right) = \lim_{z \to i\nu_n} \underbrace{\frac{(z - i\nu_n)}{e^{\beta\hbar z} - 1}}_{\delta = z - i\nu_n} = \lim_{\delta \to 0} \frac{\delta}{e^{\beta\hbar\delta} \underbrace{e^{i\nu_n\beta\hbar}}_{1} - 1} = \frac{+1}{\beta\hbar} \qquad (270.1)$$

considerar a integral:

$$I = \frac{1}{2\pi i} \oint_C dz \, n_{BE}(z) \, g(z) \, e^{z\eta} = \quad \text{curva } \underline{C} \text{ não envolve singularidades de } g(z)! \quad (*)$$

$$= \frac{1}{2\pi i} \cdot 2\pi i \sum_n \underbrace{\text{Res}\left( n_{BE}(i\nu_n) \, g(i\nu_n) \, e^{i\nu_n\eta} \right)}_{\frac{1}{\beta\hbar} g(i\nu_n) e^{i\nu_n \eta}} = I_B \qquad (270.2)$$




(270.3)

$\hookrightarrow$ soma $I_B$ pode ser escrita como:

$$I_B = \frac{1}{2\pi i} \oint_C dz \, n_{BE}(z) \, g(z) \, e^{z\eta} \quad ; \quad \eta > 0 \qquad (270.4)$$

(2) férmions:

notar:

$$n_{FD}(z) = \frac{1}{e^{\beta\hbar z}+1} \quad : \text{ polos } \beta\hbar z = (2n+1)\pi i$$

↳ $z = (2n+1)\pi i/\beta\hbar = i\omega_n$

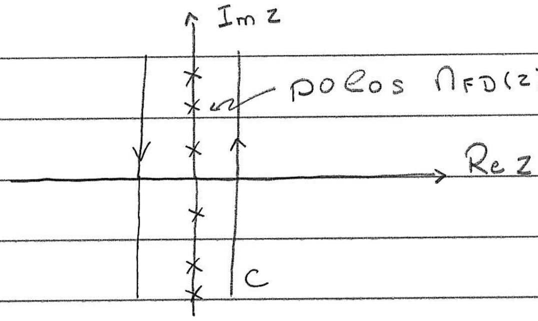
$$\text{e} \quad \underset{z=i\omega_n}{\mathrm{Res}}\left(n_{FD}(z)\right) = \lim_{z\to i\omega_n} \frac{z-i\omega_n}{\underbrace{e^{\beta\hbar z}+1}_{\delta = z-i\omega_n}} = \lim_{\delta\to 0}\frac{\delta}{e^{\beta\hbar\delta}\underbrace{e^{i\omega_n\beta\hbar}}_{=-1}+1} = -\frac{1}{\beta\hbar} \qquad (271.1)$$

considerar a integral:

$$I = \frac{-1}{2\pi i}\oint_C dz\, n_{FD}(z)\, g(z)\, e^{z\eta} \;\underset{=}{=}$$

veja (*) pg. 270

$$= \frac{-1}{2\pi i}\cdot 2\pi i \sum_n \underbrace{\mathrm{Res}\left(n_{FD}(i\omega_n)\, g(i\omega_n)\, e^{i\omega_n\eta}\right)}_{\frac{-1}{\beta\hbar}\, g(i\omega_n)\, e^{i\omega_n\eta}} = I_F \qquad (271.2)$$




(271.3)

↳ soma $I_F$ pode ser escrita como:

$$I_F = \frac{-1}{2\pi i}\oint_C dz\, n_{FD}(z)\, e^{z\eta} \quad ; \quad \eta > 0 \qquad (271.4)$$

Ex.: $g(z)$: função c/ polos simples;

considerar: $$g(z) = \frac{1}{z - x} \; ; \quad x \in \mathbb{R} \, , \; x > 0 \qquad (272.1)$$

(1) bósons:

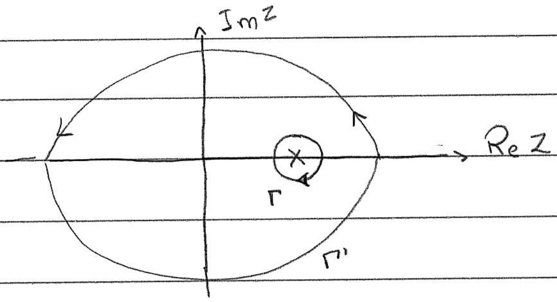
Eq. (270.4): $$I_B = \oint_C \frac{dz}{2\pi i} \, n_{BE}(z) \, . \, \frac{e^{z\eta}}{z - x} \; ;$$

podemos deformar o contorno $C \to \Gamma + \Gamma'$;
como $\oint_{\Gamma'} \to 0$ (veja abaixo), temos que:

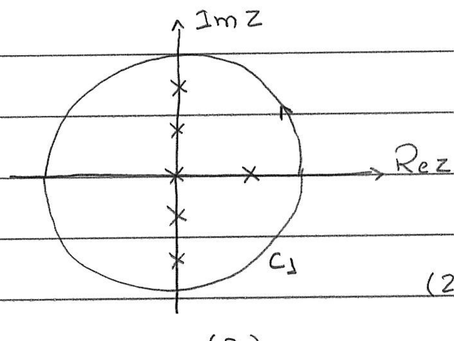
$$I_B = \oint_{\Gamma} \frac{dz}{2\pi i} \, n_{BE}(z) \, . \, \frac{e^{z\eta}}{z - x} = \frac{1}{2\pi i} \, . \, 2\pi i \, (-1) \, n_{BE}(x) \, e^{x\eta}$$

↑ CLOCKWISE

$$\xrightarrow[\eta \to 0]{} \frac{-1}{e^{\beta\hbar x} - 1}$$




(A)




(272.2)

(B)

$$\hookrightarrow \frac{1}{\beta\hbar} \sum_n \frac{1}{i\nu_n - x} \, e^{i\nu_n \eta} = I_B = \frac{-1}{e^{\beta\hbar x} - 1} \qquad (272.3)$$

· sobre a $\oint_{\Gamma'}$ :

notar : p/ $|z| \to +\infty$, o integrando de (270.4):

$$(I) = \frac{1}{e^{\beta z} - 1} \cdot \frac{e^{z\eta}}{z - x} \quad (\hbar = 1) \text{ é dado por:}$$

· $\mathrm{Re}\, z > 0$ : $(I) \sim \frac{1}{z} \cdot e^{(\eta - \beta)\mathrm{Re}\, z} \xrightarrow[|z| \to +\infty]{} 0$, pois $0 < \eta < \beta\hbar$

· $\mathrm{Re}\, z < 0$ : $(I) \sim \frac{1}{z}\, e^{\eta\, \mathrm{Re}\, z} \xrightarrow[|z| \to +\infty]{} 0$ :

: notar importância do fator $e^{i\omega_n \eta}$ :

Obs.: procedimento alternativo (Bruus): considerar o contorno $C_1$ :

como $\oint_{C_1} = 0$, temos que:

$$\oint_{C_1} \frac{dz}{2\pi i}\, n_{BE}(z)\, \frac{e^{z\eta}}{z - x} =$$

$$= \frac{1}{2\pi i} \cdot 2\pi i\, (+1) \sum_n \mathrm{Res} \underbrace{\left( n_{BE}(i\nu_n)\, \frac{e^{i\nu_n \eta}}{i\nu_n - x} \right)}_{\frac{1}{\beta\hbar} \frac{e^{i\nu_n \eta}}{i\nu_n - x}} +$$

COUNTER CLOCK

$$+ \frac{1}{2\pi i} \cdot 2\pi i\, (+1) \cdot n_{BE}(i\nu_n)\, e^{i\nu_n \eta} = 0 \quad : \text{Eq. (272.3)}$$

(2) férmions:

Eq. (271.4) : $I_F = -\oint_C \frac{dz}{2\pi i}\, n_{FD}(z)\, \frac{e^{z\eta}}{z-x} =$

$$= -\oint_{\Gamma} \frac{dz}{2\pi i}\, n_{FD}(z)\, \frac{e^{z\eta}}{z-x} = \frac{-1}{2\pi i} \cdot 2\pi i\,(-1)\, n_{FD}(x)\, e^{x\eta}$$

$$\xrightarrow[\eta \to 0]{} \frac{1}{e^{\beta\hbar x}+1}$$

$$\hookrightarrow \frac{1}{\beta\hbar}\sum_n \frac{1}{i\omega_n - x}\, e^{i\omega_n \eta} = I_F = \frac{1}{e^{\beta\hbar x}+1} \qquad (274.1)$$

em particular, autoenergia (269.2):

$$\hbar\Sigma^{(1)}(\vec{k}) = (-1)\int \frac{d^3p}{(2\pi)^3}\Big(\pm(2S+1)V(0) + V(\vec{k}-\vec{p}) \; +$$

$$+ \underbrace{\frac{1}{\beta\hbar}\sum_m \frac{1}{i\omega_m - \mathfrak{z}_{\vec{p}}/\hbar}\, e^{i\omega_m\eta}}$$

$$\frac{\mp 1}{\exp(\beta\,\mathfrak{z}_{\vec{p}}) \mp 1} = \mp\, n(\mathfrak{z}_{\vec{p}}) \begin{cases} n_{BE}(\mathfrak{z}_{\vec{p}}) \\ n_{FD}(\mathfrak{z}_{\vec{p}}) \end{cases}$$

$$= \int \frac{d^3p}{(2\pi)^3}\Big((2S+1)V(0) \pm V(\vec{k}-\vec{p})\Big)\, n(\mathfrak{z}_{\vec{p}}) \qquad (274.2)$$

Obs.: Eq. (274.2): OK p/ bósons na ausência de condensação BE!

· Eq. de Dyson,

· novamente: similaridades entre funções de Green $G$ e $\mathcal{G}$

↳ ∃ eq. de Dyson p/ formalismo $T \neq 0$!

· forma típica $\mathcal{G}$ no espaço de coordenadas (veja Eqs. (264.1) e (264.2)):

$$\mathcal{G}(1,2) = \mathcal{G}^0(1,2) + \int d^3r_3\, d^3r_4 \int_0^{\beta\hbar} d\tau_3\, d\tau_4 \, + \tag{275.1}$$

$$+ \mathcal{G}^0(1,3)\, \tilde{\Sigma}(3,4)\, \mathcal{G}^0(4,2)$$

: comparar c/ Eq. (184.1)

↑ auto energia total

similar $T=0$, é interessante introduzir a <u>autoenergia própria</u>:

$$\tilde{\Sigma}(1,2) = \Sigma(1,2) + \int d3\, d4\; \Sigma(1,3)\, \mathcal{G}^0(3,4)\, \Sigma(3,4) + \dots \tag{275.2}$$

↳ Eq. (275.1):

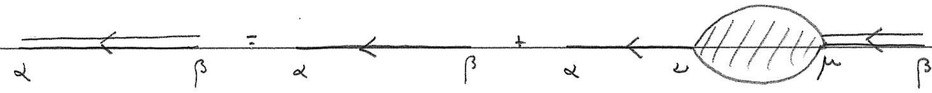
$$\mathcal{G}(1,2) = \mathcal{G}^0(1,2) + \int d3\, d4\; \mathcal{G}^0(1,3)\, \Sigma(3,4)\, \mathcal{G}(4,2) : \tag{275.3}$$

↑ autoenergia própria

: Eq. de Dyson: comparar c/ Eq. (185.3)

· novamente: p/ sistema espacialmente homogêneo, é interessante considerar a Eq. de Dyson no espaço de momento; similar Eq. (186.2), verifica-se que:

$$\mathcal{G}_{\alpha\beta}(\vec{k},\omega_n) = \mathcal{G}^0_{\alpha\beta}(\vec{k},\omega_n) + \mathcal{G}^0_{\alpha\nu}(\vec{k},\omega_n)\, \Sigma_{\nu\mu}(\vec{k},\omega_n)\, \mathcal{G}_{\mu\beta}(\vec{k},\omega_n)$$

ou  (275.4) em particular, se $\mathcal{G}_{\alpha\beta} = \delta_{\alpha\beta}\,\mathcal{G}$ , $\mathcal{G}^0_{\alpha\beta} = \delta_{\alpha\beta}\,\mathcal{G}^0$ e $\Sigma_{\alpha\beta} = \delta_{\alpha\beta}\,\Sigma$, temos que:

$$\mathcal{G}(\vec{k},\omega_n) = \mathcal{G}^0(\vec{k},\omega_n) + \mathcal{G}^0(\vec{k},\omega_n)\,\Sigma(\vec{k},\omega_n)\,\mathcal{G}(\vec{k},\omega_n)$$

(276.1)

$$\hookrightarrow \mathcal{G}(\vec{k},\omega_n) = \frac{1}{\mathcal{G}^0(\vec{k},\omega_n)^{-1} - \Sigma(\vec{k},\omega_n)}$$

⊕ Eqs. (254.1) e (254.2):

$$\mathcal{G}_{\alpha\beta}(\vec{k},\omega_n) = \frac{\delta_{\alpha\beta}}{i\omega_n - \xi_{\vec{k}}/\hbar - \Sigma(\vec{k},\omega_n)} \quad : \quad (276.2)$$

onde $\xi_{\vec{k}} = \epsilon_{\vec{k}} - \mu$ : comparar pg. 186

Obs. 1: ≠ Eq. (186.5), $\omega_n$ é uma variável discreta enquanto $\omega$ em (186.5) é uma frequência (contínua)
$\hookrightarrow$ polos (276.2) ≠ energia quasipartículas!

Obs. 2: é possível expressar a energia interna (251.1) e o potencial termodinâmico em termos da autoenergia, veja Eqs. (26.10) e (26.11), Fetter.

· similar caso $T=0$, é possível introduzir o conceito de inserção de polarização (própria);
p/ potencial de interação (265.2) independente de spin, temos que, veja Eq. (191.1):

$$U^R(\vec{q},\omega_n) = U(\vec{q},\omega_n) + U(\vec{q},\omega_n)\,\Pi(\vec{q},\omega_n)\,U^R(\vec{q},\omega_n)$$

(277.1)

$$\hookrightarrow U^R(\vec{q},\omega_n) = \frac{U(\vec{q},\omega_n)}{1 - U(\vec{q},\omega_n)\,\Pi(\vec{q},\omega_n)}$$

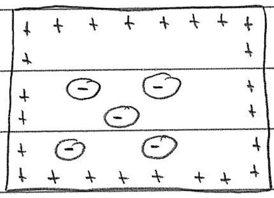
novamente, como $\omega_n$ variável discreta:

$\hookrightarrow$ $U^R(\vec{q},\omega_n) \neq$ potencial efetivo como no caso $T=0$ e procedimento distinto caso $T=0$ p/ determinação energia modos de excitação coletivos!

Ex.: Random phase approximation (RPA) - II.

ideia: descrever o gás de elétrons interagentes (jellium model, veja pg. 49) na RPA.

Lembrar modelo (49.1) e hamiltoniano (51.2):



: modelo simples p/ metal (jellium model)

$$H = \sum_{\vec{k},\alpha} \epsilon_{\vec{k}}\, c^{\dagger}_{\vec{k}\alpha} c_{\vec{k}\alpha} + \frac{1}{2V} \sum_{\substack{\vec{k},\vec{p},\vec{q}\neq 0\\ \alpha,\beta}} \frac{4\pi e^2}{q^2}\, c^{\dagger}_{\vec{k}+\vec{q}\,\alpha}\, c^{\dagger}_{\vec{p}-\vec{q}\,\beta}\, c_{\vec{p}\beta}\, c_{\vec{k}\alpha} \qquad (278.1)$$

onde $\epsilon_{\vec{k}} = \hbar^2 k^2/2m$

Lembrar Eq. (265.2):

$$U(\vec{q},\nu_n) = \int d^3r \int_0^{\beta\hbar} d\tau\, e^{-i\vec{q}\cdot\vec{r}}\, e^{i\nu_n\tau} \underbrace{U(\vec{r},\tau)}_{V(\vec{r})\,\delta(\tau)} = V(\vec{q}) \qquad (278.2)$$

Como termo $\vec{q}=0$ excluído (278.1) $\to$ diagramas c/ linhas de interação $\overset{\vec{q}=0}{- - \to - -}$ : excluídos!

· p/ a análise das propriedades de equilíbrio do sistema, é interessante considerar o potencial termodinâmico; verifica-se que (p/ detalhes, veja Eqs. (23.22), (25.27) e (26.11), Fetter):

$$\Omega = \Omega_0 \mp V(2S+1) \int_0^1 \frac{d\lambda}{\lambda} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\beta\hbar} \sum_n e^{i\omega_n\eta}\, \frac{\hbar}{2} \underbrace{\Sigma^{\lambda}(\vec{k},\omega_n)\, \mathcal{G}^{\lambda}(\vec{k},\omega_n)}_{(\mathrm{I})} \qquad (278.3)$$

onde $\Sigma^{\lambda}$ e $\mathcal{G}^{\lambda}$: associadas ao hamiltonio:

$$H(\lambda) = H_0 + \lambda V \rightarrow K(\lambda) = H(\lambda) - \mu N = H_0 - \mu N + \lambda V$$

(279.1)

notar: $H(\lambda=0) = H_0$ : sistema não-interagente
$H(\lambda=1) = H_0 + V$ : " interagente;

lembrar: $\Omega = \Omega(T, V, \mu)$;

vamos considerar spin $s = 1/2 \rightarrow (2s+1) = 2$.

· Eq. de Dyson (276.1): $\mathcal{G} = \mathcal{G}^0 + \mathcal{G}^0 \Sigma \mathcal{G}$

↳ $\mathcal{G} = \mathcal{G}^0 + \mathcal{G}^0 \Sigma \mathcal{G}^0 + \mathcal{G}^0 \Sigma \mathcal{G}^0 \Sigma \mathcal{G}^0 + \ldots$

(279.2)

e integrando (278.3):

$$(I) = \Sigma \mathcal{G} = \Sigma \mathcal{G}^0 + \Sigma \mathcal{G}^0 \Sigma \mathcal{G}^0 + \Sigma \mathcal{G}^0 \Sigma \mathcal{G}^0 \Sigma \mathcal{G}^0 + \ldots$$

· 1ª ordem:

como termo $V(\vec{q}=0)$ excluído → apenas 2º diagrama pg. 268 deve ser considerado; temos que

$$\hbar \Sigma^{(1)}(\vec{k}, \omega_n) = -\int \frac{d^3q}{(2\pi)^3} V(\vec{k}-\vec{q})\, n_{FD}(\xi_{\vec{q}}) \quad : \text{Eq. } (274.2)$$

↳ $\hbar \Sigma^{\lambda(1)}(\vec{k}, \omega_n) = -\int \frac{d^3q}{(2\pi)^3} \lambda V(\vec{k}-\vec{q})\, n(\xi_{\vec{q}})$ : veja Eq. (279.1)

↳ Eq. (278.3) c/ $\Sigma^{\lambda} = \Sigma^{\lambda(1)}$ e $\mathcal{G}^{\lambda} = \mathcal{G}^0$:

$$\Omega_1 = -V \underbrace{\int_0^1 \frac{d\lambda}{\lambda}\,.\,\lambda}_{1} \int \frac{d^3k\,d^3q}{(2\pi)^6}\, v(\vec{k}-\vec{q})\, n(3\vec{q})\, \underbrace{\frac{1}{\beta\hbar}\sum_n e^{i\omega_n \eta}\, \mathcal{G}^0(\vec{k},\omega_n)}_{=\, n(3\vec{k})}$$

Eq. (274.1)

$$= -V \int \frac{d^3k\,d^3q}{(2\pi)^6}\, v(\vec{k}-\vec{q})\, n(3\vec{q})\, n(3\vec{k}) \; : \qquad (280.1)$$

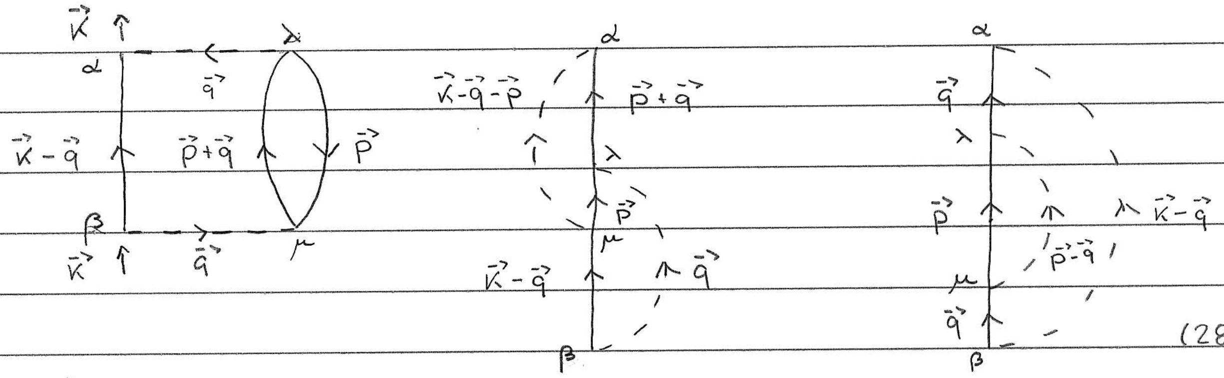
: comparar c/ caso $T=0$ Eq. (53.2)

Obs.: se $\Omega \simeq \Omega_0 + \Omega_1$ (HF approximation), verifica-se que o calor específico $C_V \sim -\frac{T}{\ln T}$, $T \to 0$ : NOT OK

c/ comportamento metais : veja P.8.1, Fetter.

· 2ª ordem:

Lembrar diagramas (176.1): diagramas 2, 3, 7, 8, 9, 10;
como termo $V(\vec{q}=0)$ excluído $\to$ apenas diagramas 2, 3 e 7
devem ser considerados;



(A) (B) (C) (280.2)

$\vec{k}, \omega_n$

$\vec{q}, \nu_l$

$\vec{p}, \omega_m$

regras (268.1):

$$\Sigma^{2A}_{\alpha\beta}(\vec{k},\omega_n) = (-1)^{F=-1} \left(\frac{-1}{\beta\hbar^2(2\pi)^3}\right)^2 \sum_{\mu,\lambda}\sum_{m,l} \int d^3q\, d^3p\; U^2(\vec{q})\, *$$

$$*\; \delta_{\alpha\beta}\, \mathcal{G}^0(\vec{k}-\vec{q}, \omega_n-\nu_l)\, \delta_{\mu\lambda}\, \mathcal{G}^0(\vec{p},\omega_m)\, \delta_{\mu\lambda}\, \mathcal{G}^0(\vec{p}+\vec{q}, \omega_m+\nu_l)$$

$\hookrightarrow \Sigma^{2A}_{\alpha\beta} = \delta_{\alpha\beta}\, \Sigma^{2A}$ e

$$\Sigma^{2A}(\vec{k}, \omega_n) = \frac{-2}{\hbar^2} \frac{1}{(\beta\hbar)^2} \sum_{m,\ell} \int \frac{d^3q\, d^3p}{(2\pi)^6}\, U^2(\vec{q})\, \mathcal{G}^0(\vec{p}, \omega_m) \times$$

$$\times\, \mathcal{G}^0(\vec{p}+\vec{q}, \omega_m + \nu_\ell)\, \mathcal{G}^0(\vec{k}-\vec{q}, \omega_n - \nu_\ell) \; ; \qquad (281.1)$$

similar $\Sigma^{2B}(\vec{k}, \omega_n)$ e $\Sigma^{2C}(\vec{k}, \omega_n)$ : veja Eq. (30.4), Fetter.

. como $U(\vec{q}) = V(\vec{q}) \propto q^{-2}$, temos que:

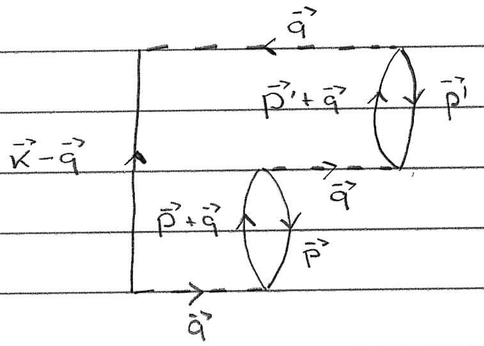
$$\Sigma^{2A} \sim \int q^2 dq \frac{1}{q^4} \to +\infty$$

$$\Sigma^{2B} \sim \int q^2 dq \frac{1}{q^2} \cdot \frac{1}{(\vec{k}-\vec{q}-\vec{p})^2} < +\infty \qquad (281.2)$$

$$\Sigma^{2C} \sim \int q^2 dq \frac{1}{(\vec{p}-\vec{q})^2} \cdot \frac{1}{(\vec{k}-\vec{q})^2} < +\infty \; :$$

: divergência $\Sigma^{2A} \sim$ presença 2 linhas de interação c/ momento $\hbar\vec{q}$ !

. similar ordem superiores;
e.g., 3ª ordem:



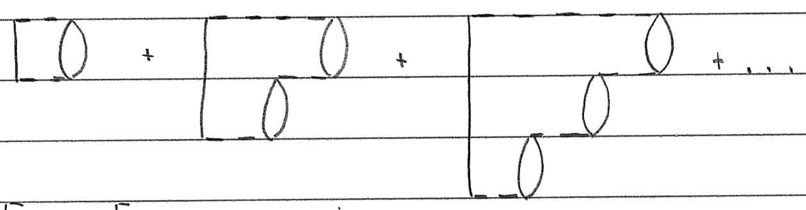
: $\Sigma^{3A} \sim \int q^2 dq \frac{1}{q^6} \to +\infty$

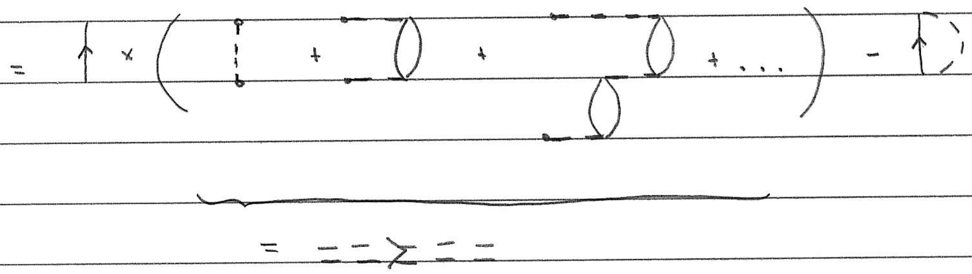
de fato, p/ cada ordem n $\exists$ diagrama $\Sigma^{nA}$ que é "mais divergente" que os demais;

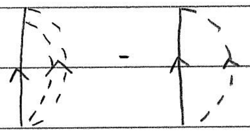
$\hookrightarrow$ proposta RPA:

$$\Sigma^{RPA} = \Sigma^{(1)} + \Sigma^{2B} + \Sigma^{2C} + \underbrace{\sum_{n\geq 2} \Sigma^{nA}}_{= \Sigma^{A}} \qquad \Sigma^{A} : \Sigma^{n}, \text{ Fetter} \qquad (282.1)$$

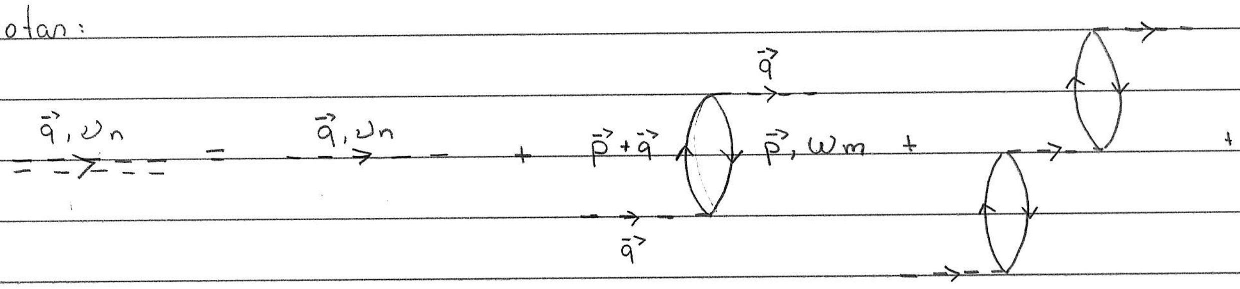
notar:

$\Sigma^A =$ 



$=$  (282.2)

notar:




$+ \ldots$

Veja Eqs. (202.4) e (203.2)

ou $U^R(\vec{q}, \nu_n) = U(\vec{q}, \nu_n) + U(\vec{q}, \nu_n)\, \pi^0(\vec{q}, \nu_n)\, U(\vec{q}, \nu_n) + \ldots$

$$= U(\vec{q}, \nu_n) + U(\vec{q}, \nu_n)\, \pi^0(\vec{q}, \nu_n)\, U^R(\vec{q}, \nu_n) \, ; \qquad (282.3)$$

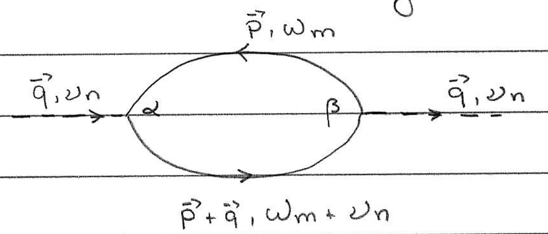
$\nu_n$ : par!

$$\hookrightarrow U^R(\vec{q},\nu_n) = \frac{U(\vec{q},\nu_n)}{1 - U(\vec{q},\nu_n)\,\Pi^0(\vec{q},\nu_n)} = \frac{V(\vec{q})}{1 - V(\vec{q})\,\Pi^0(\vec{q},\nu_n)} : \qquad (283.1)$$

∴ veja Eq. (208.1)

· sobre $\Pi^0(\vec{q},\nu_n)$:

utilizando as regras (268.1), temos que:




:

$$\therefore U^2(q,\nu_n)\sum_{\alpha\beta}(-1)^{F=1}\left(\frac{-1}{\beta\hbar^2(2\pi)^3}\right)\sum_m\int d^3p\;\delta_{\alpha\beta}\,G^0(\vec{p},\omega_m)\,*\,\delta_{\alpha\beta}\,G^0(\vec{p}+\vec{q},\omega_m+\nu_n)$$

$$= U^2(q,\nu_n)\,*$$

$$*\,\underbrace{\frac{2}{\hbar}\cdot\frac{1}{\beta\hbar}\sum_m\int\frac{d^3p}{(2\pi)^3}\,G^0(\vec{p},\omega_m)\,G^0(\vec{p}+\vec{q},\omega_m+\nu_n)}_{\Pi^0(\vec{q},\nu_n)} \qquad (283.1)$$

: comparar Eq. (202.4)

⊕ Eq. (254.2):

$$\hbar\,\Pi^0(\vec{q},\nu_n) = \frac{2}{\beta\hbar}\sum_m\int\frac{d^3p}{(2\pi)^3}\,\underbrace{\frac{1}{i\omega_m - \xi_{\vec{p}}/\hbar}\cdot\frac{1}{i\omega_m + i\nu_n - \xi_{\vec{p}+\vec{q}}/\hbar}}$$

$$\frac{1}{i\nu_n - (\xi_{\vec{p}+q} - \xi_{\vec{p}})/\hbar}\,*\left(\underbrace{\frac{1}{i\omega_m - \xi_{\vec{p}}/\hbar}}_{(\mathrm{I})} - \underbrace{\frac{1}{i\omega_m + i\nu_n - \xi_{p+q}/\hbar}}_{(\mathrm{II})}\right)$$

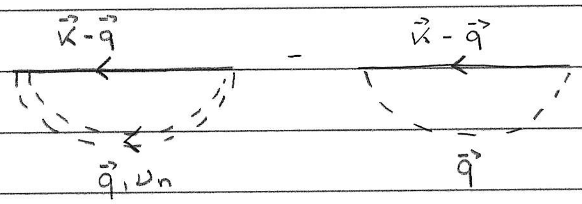
Eq. (274.1) : $\frac{1}{\beta\hbar}\sum_m e^{i\omega_m \eta}\,(\mathrm{I}) = n_{FD}(\xi_{\vec p})$

$$\frac{1}{\beta\hbar}\sum_m e^{i\omega_m \eta}\,(\mathrm{II}) = n_{FD}(\xi_{\vec p+\vec q})$$

↳ $\hbar\Pi^0(\vec q,\nu_n) = -2\int\frac{d^3p}{(2\pi)^3}\cdot\frac{n(\xi_{\vec p+\vec q}) - n(\xi_{\vec p})}{i\nu_n - (\xi_{\vec p+\vec q}-\xi_{\vec p})/\hbar}$ (283.2)

· sobre a autoenergia $\Sigma^A(\vec k,\omega_n)$:

Eq. (282.2) ⊕ regras (268.1):

$\Sigma^A(\vec k,\omega_m) =$ 


$$= \frac{-1}{\hbar}\cdot\frac{1}{\beta\hbar}\sum_n\int\frac{d^3q}{(2\pi)^3}\underbrace{\left(U^R(\vec q,\nu_n) - U(\vec q,\nu_n)\right)}_{\frac{V^2(\vec q)\,\Pi^0(\vec q,\nu_n)}{1-V(\vec q)\,\Pi^0(\vec q,\nu_n)}}\mathcal{G}^0(\vec k-\vec q,\omega_m-\nu_n)$$

↳ $\hbar\Sigma^A(\vec k,\omega_m) = \frac{-1}{\beta\hbar}\sum_n\int\frac{d^3q}{(2\pi)^3}\,\frac{V^2(\vec q)\,\Pi^0(\vec q,\nu_n)}{1-V(\vec q)\,\Pi^0(\vec q,\nu_n)}\,\mathcal{G}^0(\vec k-\vec q,\omega_m-\nu_n)$

$< +\infty$ ! (283.4)

· sobre o potencial termodinâmico,

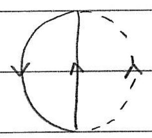
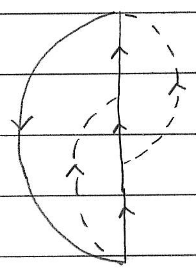
Eqs. (278.3), (279.2) e (282.1) → integrando Eq. (278.3):

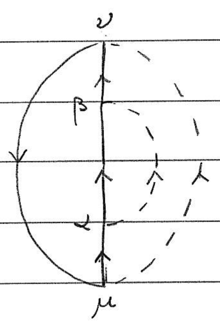
$$(I) = \Sigma^{RPA} g = \Sigma^{RPA} g^0 + \Sigma^{RPA} g^0 \Sigma^{RPA} g^0 + \dots$$

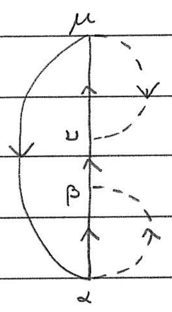
$$= \Sigma^{(1)} g^0 + \Sigma^{2B} g^0 + \Sigma^{2C} g^0 + \Sigma^{A} g^0 + \Sigma^{(1)} g^0 \Sigma^{(1)} g^0 + \dots$$

↳ $\Omega \simeq \Omega_0 + \Omega_1 + \Omega_{2B} + \Omega_{2C} + \Omega_A + \Omega_{2D}$ (283.5)

notar:

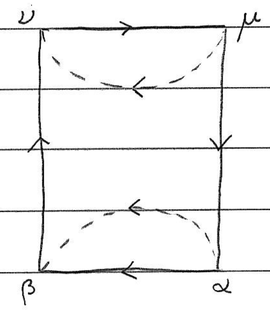
$\Omega_1$ :  : Eq. (280.1) $\Omega_{2B}$ : 

$\Omega_{2C}$ : 


$\Omega_{2D}$ : 


de fato, $\Omega_{2C}$ e $\Omega_{2D}$ são topologicamente equivalentes:

comparar c/




↳ $\Omega \simeq \Omega_0 + \Omega_1 + \Omega_{2B} + 2\Omega_{2C}$

verifica-se que:

$$\Omega_{2B}(T,V,\mu) = V \int \frac{d^3k\, d^3p\, d^3q}{(2\pi)^9} \cdot V(\vec{q})\, V(\vec{k}+\vec{p}+\vec{q})\, n(\beta\vec{k})\, n(\beta\vec{p}) \, *$$

$$* \, \frac{(1-n(\beta\vec{k}+\vec{q}))(1-n(\beta\vec{p}+\vec{q}))}{\epsilon_{\vec{k}+\vec{q}} + \epsilon_{\vec{p}+\vec{q}} - \epsilon_{\vec{k}} - \epsilon_{\vec{p}}}$$

e

(283.6)

$$\Omega_{2C}(T,V,\mu) = -\frac{1}{2} V\beta \int \frac{d^3k\, d^3p\, d^3q}{(2\pi)^9} \, V(\vec{k}-\vec{q})\, V(\vec{p}-\vec{q}) \, *$$

$$* \, n(\beta\vec{k})\, n(\beta\vec{p})\, n(\beta\vec{q})\, (1 - n(\beta\vec{q}))$$

· Eqs. (278.3) e (283.4):

$$\Omega_A = 2V \int_0^1 \frac{d\lambda}{\lambda} \int \frac{d^3k}{(2\pi)^3} \cdot \frac{1}{\beta\hbar} \sum_m e^{i\omega_m \eta} \frac{\hbar}{2} \Sigma^\lambda(\vec{k},\omega_m)\, \mathcal{G}^0(\vec{k},\omega_m)$$

$$= -V \frac{1}{\beta\hbar} \sum_n \int \frac{d^3q}{(2\pi)^3} \int_0^1 \frac{d\lambda}{\lambda} \cdot \frac{\lambda^2 V^2(\vec{q})\, \pi^0(\vec{q},\nu_n)}{1-\lambda V(\vec{q})\, \pi^0(\vec{q},\nu_n)} \, *$$

$$* \, \underbrace{\frac{1}{\beta\hbar} \sum_m e^{i\omega_m \eta} \int \frac{d^3k}{(2\pi)^3} \mathcal{G}^0(\vec{k}-\vec{q},\omega_m-\nu_n)\, \mathcal{G}^0(\vec{k},\omega_m)}_{=\,\hbar/2\ \pi^0(\vec{q},\nu_n)}$$

$$= -V \cdot \frac{\hbar}{2} \frac{1}{\beta\hbar} \sum_n \int \frac{d^3q}{(2\pi)^3} \underbrace{\int_0^1 \frac{d\lambda}{\lambda} \frac{\lambda^2 (V(\vec{q})\, \pi^0(\vec{q},\nu_n))^2}{1-\lambda V(\vec{q})\, \pi^0(\vec{q},\nu_n)}}_{(-1)\left(\ln\left(1 - V(\vec{q})\pi^0(\vec{q},\nu_n)\right) + V(\vec{q})\pi^0(\vec{q},\nu_n)\right)}$$

(283.7)

· é interessante determinar as contribuições (283.6) e (283.7) p/ o gás de elétrons no limite $T \to 0$;
de fato, nesse caso, verifica-se que a energia do estado fundamental assume a forma (p/ detalhes, veja Sec. 30, Fetter):

$$\underset{\substack{\uparrow \\ \text{sistema} \\ \text{não-interagente}}}{E_{GS} = E_0} + \Omega_1(\epsilon_F^0) + \underbrace{\Omega_A(\epsilon_F^0) + \Omega_{2B}(\epsilon_F^0)}_{E_{CORR}},$$

termo de troca (53.2)

onde $\epsilon_F^0 = \mu_0(n) = \hbar^2 k_F^2/2m$ : energia de Fermi, sistema não-interagente.

e a energia de correlação:

$$E_{CORR} = \frac{e^2}{2a_0}\left(0.0622 \ln r_s - 0.094 + O(r_s \ln r_s)\right) : \qquad (283.8)$$

: comparar c/ Eq. (54.2)

· Detalhes Eq. (283.6):

Diagrama (280.2) ⊕ regras (268.1):

$$\Sigma^{2B}_{\alpha\beta}(\vec{k},\omega_n) = \left(\frac{-1}{\beta\hbar^2(2\pi)^3}\right)^2 \sum_{\mu,\lambda}\sum_{m,l}\int d^3q\, d^3p\; U(\vec{q})\,U(\vec{k}-\vec{q}-\vec{p})\,*$$

$$* \; G^0(\vec{k}-\vec{q},\omega_n-\nu_l)\, G^0(\vec{p},\omega_m)\, G^0(\vec{p}+\vec{q},\omega_m+\nu_l)\,\delta_{\mu\beta}\,\delta_{\mu\lambda}\,\delta_{\lambda\alpha}$$

↳ Eq. (278.3):

$$\Omega_{2B} = 2V\underbrace{\int_0^1 \frac{d\lambda}{\lambda}\cdot\lambda^2}_{=1/2}\; \frac{1}{(\beta\hbar)^3}\,(-1)^2\cdot\frac{1}{\hbar^2}\sum_{n,m,l} e^{i\omega_n\eta}\int\frac{d^3q\,d^3p\,d^3k}{(2\pi)^9} * \frac{\hbar}{2}$$

$$* \; V(\vec{q})\cdot V(\vec{k}-\vec{q}-\vec{p})\, *$$

$$* \; \underbrace{G^0(\vec{k},\omega_n)\, G^0(\vec{k}-\vec{q},\omega_n-\nu_l)\, G^0(\vec{p},\omega_m)\, G^0(\vec{p}+\vec{q},\omega_m+\nu_l)}_{\frac{1}{i\omega_n-\xi_{\vec{k}}/\hbar}\cdot\frac{1}{i\omega_n-i\nu_l-\xi_{\vec{k}-\vec{q}}/\hbar}\cdot\frac{1}{i\omega_m-\xi_{\vec{p}}/\hbar}\cdot\frac{1}{i\omega_m+i\nu_l-\xi_{\vec{p}+\vec{q}}/\hbar}}$$

Como:

· $$\frac{1}{\beta\hbar}\sum_n e^{i\omega_n\eta}\, G^0(\vec{k},\omega_n)\, G^0(\vec{k}-\vec{q},\omega_n-\nu_l) = -\frac{\left(n(\xi_{\vec{k}-\vec{q}})-n(\xi_{\vec{k}})\right)}{-i\nu_l-(\xi_{\vec{k}-\vec{q}}-\xi_{\vec{k}})/\hbar}$$

Veja Eq. (283.2)

· $$\frac{1}{\beta\hbar}\sum_m G^0(\vec{p},\omega_m)\, G^0(\vec{p}+\vec{q},\omega_m+\nu_l) = -\frac{\left(n(\xi_{\vec{p}+\vec{q}})-n(\xi_{\vec{p}})\right)}{i\nu_l-(\xi_{\vec{p}+\vec{q}}-\xi_{\vec{p}})/\hbar}$$

· $$\frac{1}{\beta\hbar}\sum_l \frac{1}{i\nu_l-(\xi_{\vec{k}}-\xi_{\vec{k}-\vec{q}})/\hbar}\cdot\frac{1}{i\nu_l-(\xi_{\vec{p}+\vec{q}}-\xi_{\vec{p}})/\hbar} = (I)$$

$$(I) = \frac{1}{(\xi_{\vec{k}} - \xi_{\vec{k}-\vec{q}})/\hbar - (\xi_{\vec{p}+\vec{q}} - \xi_{\vec{p}})/\hbar} \cdot \frac{1}{\beta\hbar} \sum_{l} e^{i\nu_l \eta} \,*$$

$$* \left( \frac{1}{i\nu_l - (\xi_{\vec{k}} - \xi_{\vec{k}-\vec{q}})/\hbar} - \frac{1}{i\nu_l - (\xi_{\vec{p}+\vec{q}} - \xi_{\vec{p}})/\hbar} \right)$$

$$= (-1) \left( n_{BE}(\xi_{\vec{k}} - \xi_{\vec{k}-\vec{q}}) - n_{BE}(\xi_{\vec{p}+\vec{q}} - \xi_{\vec{p}}) \right)$$

Eq. (272.3)

$$\hookrightarrow \Omega_{2B} = \frac{1}{2} V \int \frac{d^3k\, d^3q\, d^3p}{(2\pi)^9} * V(\vec{q})\, V(\vec{k}-\vec{q}-\vec{p}) \cdot \frac{1}{\epsilon_{\vec{k}-\vec{q}} + \epsilon_{\vec{p}+\vec{q}} - \epsilon_{\vec{k}} - \epsilon_{\vec{p}}} \,*$$

$$* (-1) * (n_{\vec{k}-\vec{q}} - n_{\vec{k}})(n_{\vec{p}+\vec{q}} - n_{\vec{p}})\left(n_{BE}(\xi_{\vec{k}} - \xi_{\vec{k}-\vec{q}}) - n_{BE}(\xi_{\vec{p}+\vec{q}} - \xi_{\vec{p}})\right)$$

$\vec{q} \to -\vec{q}$ e $\vec{p} \to -\vec{p}$

$$\hookrightarrow \Omega_{2B} = \frac{1}{2} V \int \frac{d^3k\, d^3q\, d^3p}{(2\pi)^9} \cdot V(\vec{q})\, V(\vec{k}+\vec{p}+\vec{q}) \cdot \frac{1}{\epsilon_{\vec{k}+\vec{q}} + \epsilon_{\vec{p}+\vec{q}} - \epsilon_{\vec{k}} - \epsilon_{\vec{p}}} \,*$$

$$* (-1) * (n_{\vec{k}+\vec{q}} - n_{\vec{k}})(n_{\vec{p}+\vec{q}} - n_{\vec{p}})\left(n_{BE}(\xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}}) - n_{BE}(\xi_{\vec{p}+\vec{q}} - \xi_{\vec{p}})\right)$$

· Função de Green a tempo real.

Lembrar $T=0$:

· polos $G(\vec{k},\omega)$: energia e tempo de vida quase partícula =

= estado excitado $\pm 1$ partícula;

· $D^R(\vec{k},\omega)$: blindagem ~ impureza em um gás de elétrons, espectro modos coletivos, e.g., oscilações de plasma.

$\neq$ p/ $\mathcal{G}(\vec{k},\omega)$: nesse caso, é necessário introduzir a função de Green a tempo real!

· Similar Eq. (244.1)

↳ Definição: função de Green a tempo real

$$i\bar{G}_{\alpha\beta}(\vec{r},t;\vec{r}',t') = \frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta K}\,T\left(\psi_\alpha(\vec{r},t)\,\psi^+_\beta(\vec{r}',t')\right)\right]. \quad (284.1)$$

onde $\psi_\alpha(\vec{r},t) = \psi_{H\alpha}(\vec{r},t)$ : op. de campo

$= e^{iKt/\hbar}\,\psi_\alpha(\vec{r})\,e^{-iKt/\hbar}$ versão de Heisenberg

notar: $\bar{G} \propto \vec{r},t;\vec{r}',t';T$ e $\mu$!

· se $H \neq H(t) \rightarrow \bar{G}_{\alpha\beta}(\vec{r},\vec{r}',t-t')$

⊕ p/ sistema homogêneo: $\bar{G}_{\alpha\beta}(\vec{r}-\vec{r}';t-t')$ (284.2)

⊕ ausência campo $\vec{B}$ e FM: $\bar{G}_{\alpha\beta} = \delta_{\alpha\beta}\bar{G}_\alpha$;

: apenas hipóteses que simplificam a análise!

· Eq. (284.1) p/ $t > 0$:

$$i G^{>}_{\alpha}(\vec{r},t) = \frac{1}{Z} \operatorname{Tr}\left[ e^{-\beta K} \psi_{\alpha}(\vec{r},t) \psi^{\dagger}_{\alpha}(0,0) \right] \tag{285.1}$$

Lembrar Eq. (141.1):

$$\psi_{\alpha}(\vec{r},t) = e^{-i\vec{P}\cdot\vec{r}/\hbar} \psi_{\alpha}(\vec{r}=0)\, e^{i\vec{P}\cdot\vec{r}/\hbar} \;;$$

p/ sistema homogêneo: $[H,\vec{P}] = [K,\vec{P}] = 0$

$$\hookrightarrow \psi_{\alpha}(\vec{r},t) = e^{-i\vec{P}\cdot\vec{r}/\hbar} e^{iKt/\hbar} \psi_{\alpha}(0)\, e^{-iKt/\hbar} e^{i\vec{P}\cdot\vec{r}/\hbar} \tag{285.2}$$

(+) Eq. (285.1):

$$i G^{>}_{\alpha}(\vec{r},t) = \frac{1}{Z} \operatorname{Tr}\left[ e^{-\beta K} e^{-i\vec{P}\cdot\vec{r}/\hbar} e^{iKt/\hbar} \psi_{\alpha}(0)\, e^{-iKt/\hbar} e^{i\vec{P}\cdot\vec{r}/\hbar} \psi^{\dagger}_{\alpha}(0) \right] \tag{285.3}$$

como $[H,\vec{P}] = [H,N] = [N,\vec{P}] = 0$, o $\operatorname{Tr}[\ldots]$ pode ser calculado c/ a base:

$$K|n\rangle = K_n|n\rangle = (E_n - \mu N_n)|n\rangle, \tag{285.4}$$
$$\vec{P}|n\rangle = \vec{p}_n|n\rangle.$$

temos que:

$$i G^{>}_{\alpha}(\vec{r},t) = \frac{1}{Z}\sum_{n,m} e^{-\beta K_m} e^{-i\vec{p}_m\cdot\vec{r}/\hbar} e^{iK_m t/\hbar} \langle m|\psi_{\alpha}(0)|n\rangle \,+$$
$$+\, e^{-iK_n t/\hbar} e^{i\vec{p}_n\cdot\vec{r}/\hbar} \langle n|\psi_{\alpha}(0)|m\rangle$$

$$= \frac{1}{Z}\sum_{n,m} e^{-\beta K_m} e^{i(\vec{p}_n-\vec{p}_m)\cdot\vec{r}/\hbar} e^{-i(K_n-K_m)t/\hbar} |\langle m|\psi_{\alpha}(0)|n\rangle|^2 \tag{285.5}$$

· similar p/ $t<0$ (verificar):

$i\,G^{<}_{\alpha}(\vec{r},t) =$

$$= \pm \frac{1}{Z} \sum_{n,m} e^{-\beta K_n} e^{i(\vec{p}_n - \vec{p}_m)\cdot\vec{r}/\hbar} e^{-i(K_n - K_m)t/\hbar} \,|\langle m|\psi_\alpha(0)|n\rangle|^2 \qquad (286.1)$$

Dessa forma: $\bar{G}_\alpha(\vec{r},t) = \Theta(t)\,G^{>}_{\alpha}(\vec{r},t) + \Theta(-t)\,G^{<}_{\alpha}(\vec{r},t)$

· similar Eq. (142.2), temos que

$$\bar{G}_\alpha(\vec{k},\omega) = \int d^3r\,dt\; e^{-i\vec{k}\cdot\vec{r} + i\omega t}\,\bar{G}_\alpha(\vec{r},t)$$

é dada por (veja pg. 286.1):

$$\bar{G}_\alpha(\vec{k},\omega) = \frac{1}{Z}\sum_{n,m} (2\pi)^3\,\delta\big(\vec{k} - (\vec{p}_n - \vec{p}_m)/\hbar\big)\,|\langle m|\psi_\alpha(0)|n\rangle|^2 \,\ast$$

$$\ast\left(\frac{e^{-\beta K_m}}{\omega - (K_n - K_m)/\hbar + i\eta} \mp \frac{e^{-\beta K_n}}{\omega - (K_n - K_m)/\hbar - i\eta}\right) \qquad (286.2)$$

notar:

polos $\bar{G}$ no plano $\mathrm{Re}\,\omega$ - $\mathrm{Im}\,\omega$: $\hbar\omega = K_n - K_m = E_n - E_m - \mu(N_n - N_m)$;

resíduos $\bar{G} \neq 0$ se $\langle m|\psi(0)|n\rangle \neq 0 \rightarrow N_n = N_m + 1$

e Eq. (286.2): generalização Eq. (142.3)!

· Lembrar identidade (146.2):

$$\frac{1}{\omega \pm i\eta} = P\frac{1}{\omega} \mp i\pi\,\delta(\omega)\;; \quad \omega \in \mathbb{R}$$

· Detalhes Eq. (286.2):

$$\bar{G}_\alpha(\vec{k},\omega) = \frac{1}{Z} \sum_{n,m} \underbrace{\int d^3r \, e^{-i(\vec{k}-(\vec{p}_n-\vec{p}_m)/\hbar)\cdot\vec{r}}}_{(2\pi)^3 \delta\left(\vec{k}-(\vec{p}_n-\vec{p}_m)/\hbar\right)} *$$

$$* \, |\langle m|\psi_\alpha(0)|n\rangle|^2 \, *$$

$$* \left( \underbrace{\int_0^\infty dt \, (-i) \, e^{i(\omega-(K_n-K_m)/\hbar)t} \, e^{-\eta t}}_{\frac{(-i)(-1)}{i(\omega-(K_n-K_m)/\hbar)-\eta} \cdot \frac{(-i)}{(-i)}} \, e^{-\beta K_m} + \right.$$

$$\left. + \underbrace{\int_{-\infty}^0 dt \, (-i)(\pm 1) \, e^{i(\omega-(K_n-K_m)/\hbar)t} \, e^{+\eta t}}_{\frac{(\mp i)}{i(\omega-(K_n-K_m)/\hbar)+\eta} \cdot \frac{(-i)}{(-i)}} \right)$$

↳ Eq. (286.2) p/ $\omega \in \mathbb{R}$:

$$\bar{G}_\alpha(\vec{k},\omega) = \frac{1}{Z}\sum_{n,m}(2\pi)^3\,\delta\left(\vec{k}-(\vec{p}_n-\vec{p}_m)/\hbar\right)|\langle m|\psi_\alpha(0)|n\rangle|^2 \,*$$

$$*\left(\underbrace{e^{-\beta K_m}\,\mathcal{P}\frac{1}{\omega-(K_n-K_m)/\hbar} \mp e^{-\beta K_n}\,\mathcal{P}\frac{1}{\omega-(K_n-K_m)/\hbar}}_{e^{-\beta K_m}\,\mathcal{P}\frac{1\mp e^{-\beta(K_n-K_m)}}{\omega-(K_n-K_m)/\hbar}} +\right.$$

$$\left.\underbrace{-i\pi e^{-\beta K_m}\,\delta\left(\omega-(K_n-K_m)/\hbar\right) \mp i\pi e^{-\beta K_n}\,\delta\left(\omega-(K_n-K_m)/\hbar\right)}_{-i\pi e^{-\beta K_m}\,\delta\left(\omega-(K_n-K_m)/\hbar\right)\left(1\pm e^{-\beta(K_n-K_m)/\hbar}\right)}\right)$$

(287.1)

notar: $\mathrm{Im}\,\bar{G}_\alpha(\vec{k},\omega)$ pode ser escrito como:

$$\mathrm{Im}\,\bar{G}_\alpha(\vec{k},\omega) = \frac{-\pi}{Z}\sum_{n,m}(2\pi)^3\,\delta\left(\vec{k}-(\vec{p}_n-\vec{p}_m)/\hbar\right)|\langle m|\psi_\alpha(0)|n\rangle|^2 \,*$$

$$*\,\delta\left(\omega-(K_n-K_m)/\hbar\right)\left(1\pm e^{-\beta\hbar\omega}\right)$$

(287.2)

↳ $$\mathrm{Re}\,\bar{G}_\alpha(\vec{k},\omega) = -\mathcal{P}\int_{-\infty}^{+\infty}\frac{d\omega'}{\pi}\cdot\frac{\mathrm{Im}\,G_\alpha(\vec{k},\omega')}{\omega-\omega'}\cdot\frac{1\mp e^{-\beta\hbar\omega'}}{1\pm e^{-\beta\hbar\omega'}}$$

· similar Eq. (148.3), é interessante introduzir as funções de Green retardada e avançada:

$$i\bar{G}^{R}_{\alpha\beta}(\vec{r},t;\vec{r}',t') = \theta(t-t')\,\frac{1}{Z}\,Tr\left(e^{-\beta K}\left[\psi_\alpha(\vec{r},t);\psi^\dagger_\beta(\vec{r}',t')\right]_\mp\right)$$

$$i\bar{G}^{A}_{\alpha\beta}(\vec{r},t;\vec{r}',t') = -\theta(t'-t)\,\frac{1}{Z}\,Tr\left(e^{-\beta K}\left[\psi_\alpha(\vec{r},t);\psi^\dagger_\beta(\vec{r}',t')\right]_\mp\right)$$

notar comutador/anticomutador (288.1)

· similar Eq. (286.2) e considerando as hipóteses (284.2), verifica-se que:

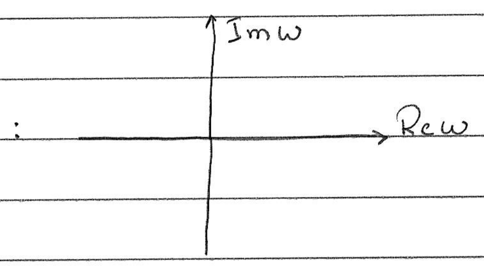
$$\bar{G}^{R,A}_{\alpha}(\vec{k},\omega) = \frac{1}{Z}\sum_{n,m} e^{-\beta K_m}(2\pi)^3\,\delta\left(\vec{k}-(\vec{p}_n-\vec{p}_m)/\hbar\right)\,|\langle m|\psi_\alpha(0)|n\rangle|^2 \,*$$

$$* \,\frac{1\mp e^{-\beta(K_n-K_m)}}{\omega-(K_n-K_m)/\hbar \pm i\eta} \qquad (288.2)$$

polos $\bar{G}^R$ : $\hbar\omega = (K_n-K_m)-i\hbar\eta$ : analítica semi-plano superior;

$\bar{G}^A$ : $\hbar\omega = (K_n-K_m)+i\hbar\eta$ : " " inferior.

:




· é interessante introduzir $\rho_\alpha(\vec{k},\omega)$, tal que:

$$\text{Im}\,\bar{G}^R_\alpha(\vec{k},\omega) = -1/2\,\rho_\alpha(\vec{k},\omega)$$

(288.3)

$$\text{e}\quad \text{Im}\,\bar{G}^A_\alpha(\vec{k},\omega) = +1/2\,\rho_\alpha(\vec{k},\omega)$$

onde

$$\rho_\alpha(\vec{k},\omega) = 2\pi \cdot \frac{1}{Z} \sum_{n,m} e^{-\beta K_m} \delta\left(\vec{k} - (\vec{p}_n - \vec{p}_m)/\hbar\right) |\langle m| \psi_\alpha(0) |n\rangle|^2 \, *$$

$$* \, \delta(\omega - (K_n - K_m)/\hbar) \left(1 \mp e^{-\beta\hbar\omega}\right) \qquad (289.1)$$

notar: Eq. (288.2) pode ser escrito como:

$$\bar{G}_\alpha^{R,A}(\vec{k},\omega) = \int \frac{d\omega'}{2\pi} \cdot 2\pi \frac{1}{Z} \sum_{n,m} e^{-\beta K_m} (2\pi)^3 \delta\left(\vec{k} - (\vec{p}_n - \vec{p}_m)/\hbar\right) *$$

$$* \, |\langle m| \psi_\alpha(0) |n\rangle|^2 \delta(\omega' - (K_n - K_m)/\hbar) \frac{(1 \mp e^{-\beta\hbar\omega'})}{\omega - \omega' \pm i\eta}$$

$$\hookrightarrow \bar{G}_\alpha^R(\vec{k},\omega) = \int \frac{d\omega'}{2\pi} \cdot \frac{\rho_\alpha(\vec{k},\omega')}{\omega - \omega' + i\eta} = -\int \frac{d\omega'}{\pi} \cdot \frac{\operatorname{Im} \bar{G}_\alpha^R(\vec{k},\omega')}{\omega - \omega' + i\eta}$$

$$(289.2)$$

$$\bar{G}_\alpha^A(\vec{k},\omega) = \int \frac{d\omega'}{2\pi} \cdot \frac{\rho_\alpha(\vec{k},\omega')}{\omega - \omega' - i\eta} = +\int \frac{d\omega'}{\pi} \cdot \frac{\operatorname{Im} \bar{G}_\alpha^A(\vec{k},\omega)}{\omega - \omega' - i\eta}$$

· Definição:

$$\Gamma_\alpha(\vec{k},z) = \int \frac{d\omega'}{2\pi} \cdot \frac{\rho_\alpha(\vec{k},\omega')}{z - \omega'} \quad ; \quad z \in \mathbb{C} \qquad (289.3)$$

$$\hookrightarrow \bar{G}_\alpha^R(\vec{k},\omega) = \Gamma_\alpha(\vec{k},\omega + i\eta)$$

$$(289.4)$$

$$\bar{G}_\alpha^A(\vec{k},\omega) = \Gamma_\alpha(\vec{k},\omega - i\eta)$$

· Eqs. (287.2) e (289.1): verifica-se que:

$$\mathrm{Im}\,\bar{G}_\alpha(\vec{k},\omega) = -\frac{1}{2}\,\rho_\alpha(\vec{k},\omega)\,\underbrace{\frac{(1 \pm e^{-\beta\hbar\omega})}{(1 \mp e^{-\beta\hbar\omega})}}_{\mathrm{tgh}\,(+\beta\hbar\omega/2)^{\mp 1}} \qquad (290.1)$$

e $\mathrm{Re}\,\bar{G}_\alpha(\vec{k},\omega) = P\int \frac{d\omega'}{2\pi}\,\frac{\rho_\alpha(\vec{k},\omega')}{\omega-\omega'}$

notar Eqs. (288.3), (289.2) e (290.1):

$$\begin{aligned} \mathrm{Re}\,\bar{G} &= \mathrm{Re}\,\bar{G}^R = \mathrm{Re}\,\bar{G}^A \\ \mathrm{Im}\,\bar{G}^R &= \mathrm{tgh}\,(\beta\hbar\omega/2)^{\pm 1}\,\mathrm{Im}\,\bar{G} \\ \mathrm{Im}\,\bar{G}^A &= -\mathrm{tgh}\,(\beta\hbar\omega/2)^{\pm 1}\,\mathrm{Im}\,\bar{G} \end{aligned} \qquad (290.2)$$

: comparar c/ Eq. (148.1)

· propriedades da função $\rho_\alpha(\vec{k},\omega)$:

(i) $\mathrm{sgn}(\omega)\,\rho_\alpha(\vec{k},\omega) \geq 0$ : bósons

$\rho_\alpha(\vec{k},\omega) \geq 0$ : férmions

(ii) $\int \frac{d\omega'}{2\pi}\,\rho_\alpha(\vec{k},\omega) = 1$ : (290.3)

: p/ detalhes, veja Eqs. (31.29) e (31.30), FetWa.

Eqs. (289.2) e (290.3)

$\hookrightarrow \bar{G}^R_\alpha(\vec{k},\omega) = \bar{G}^A_\alpha(\vec{k},\omega) \sim \frac{1}{\omega}\int \frac{d\omega'}{2\pi}\rho_\alpha(\vec{k},\omega') \sim \frac{1}{\omega}$ ; $|\omega| \to +\infty$ :

(291.1)

: comparar Eq. (147.1)

· próxima etapa: representação de Lehmann p/ a função de Green de tempo imaginário.

Eq. (244.1) ⊕ hipóteses (284.2):

$$\mathcal{G}_\alpha(\vec{r},\tau) = -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta K}\psi_\alpha(\vec{r},\tau)\psi^\dagger_\alpha(0)\right]$$

$$= -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta K} e^{-i\vec{p}\cdot\vec{r}/\hbar} e^{K\tau/\hbar}\psi_\alpha(0) e^{-K\tau/\hbar} e^{i\vec{p}\cdot\vec{r}/\hbar}\psi^\dagger_\alpha(0)\right]$$

↑ Eq. (285.2) ⊕ $it \to \tau$

$$= -\frac{1}{Z}\sum_{n,m} e^{-\beta K_m} e^{i(\vec{p}_n-\vec{p}_m)\cdot\vec{r}/\hbar} e^{-(K_n-K_m)\tau/\hbar} |\langle m|\psi_\alpha(0)|n\rangle|^2$$

↑ veja Eq. (285.5)

(291.2)

Transformada de Fourier (248.2):

$$\mathcal{G}_\alpha(\vec{k},\omega_n) = \int_0^{\beta\hbar} d\tau \int d^3r\, e^{-i\vec{k}\cdot\vec{r}} e^{i\omega_n\tau}\,\mathcal{G}_\alpha(\vec{r},\tau)$$

$$= -\frac{1}{Z}\sum_{n,m} e^{-\beta K_m} \underbrace{\int d^3r\, e^{-i(\vec{k}-(\vec{p}_n-\vec{p}_m)/\hbar)\cdot\vec{r}}}_{(2\pi)^3\,\delta(\vec{k}-(\vec{p}_n-\vec{p}_m)/\hbar)} |\langle m|\psi_\alpha(0)|n\rangle|^2 \,*$$

$$* \underbrace{\int_0^{\beta\hbar} d\tau\, \exp\left(-(K_n-K_m)/\hbar + i\omega_n\right)\tau}_{(I)}$$

Como (I) = $\dfrac{-1}{-(K_n-K_m)/\hbar + i\omega_n} \cdot \left( \underbrace{e^{i\beta\hbar\omega_n}}_{\pm 1} e^{-\beta(K_n-K_m)} - 1 \right)$

$$\hookrightarrow G_\alpha(\vec{k},\omega_n) = \frac{1}{Z} \sum_{n,m} e^{-\beta K_m} (2\pi)^3 \delta\left(\vec{k} - (\vec{p}_n - \vec{p}_m)/\hbar\right) |\langle m|\psi_\alpha(0)|n\rangle|^2 \, *$$

$$* \, \frac{1 \mp e^{-\beta(K_n-K_m)}}{i\omega_n - (K_n-K_m)/\hbar} \qquad (292.1)$$

Ou

$$G_\alpha(\vec{k},\omega_n) = \int \frac{d\omega'}{2\pi} \, 2\pi \frac{1}{Z} \sum_{n,m} e^{-\beta K_m} (2\pi)^3 \delta\left(\vec{k} - (\vec{p}_n - \vec{p}_m)/\hbar\right) \, *$$

$$* \, |\langle m|\psi_\alpha(0)|n\rangle|^2 \delta\left(\omega' - (K_n-K_m)/\hbar\right) \frac{1 \mp e^{-\beta\hbar\omega'}}{i\omega_n - \omega'}$$

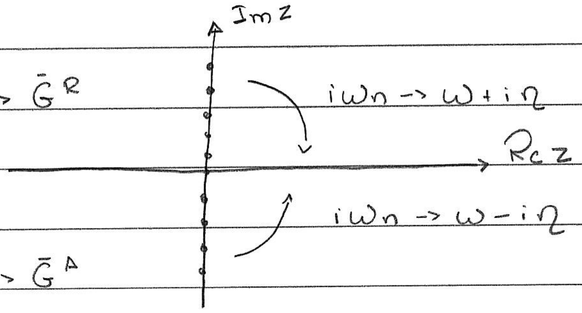
$$\hookrightarrow G_\alpha(\vec{k},\omega_n) = \int \frac{d\omega'}{2\pi} \frac{\rho_\alpha(\vec{k},\omega')}{i\omega_n - \omega'} = \Gamma_\alpha(\vec{k}, i\omega_n) \qquad (292.2)$$

notar Eqs. (289.4) e (292.2):

$G_\alpha(\vec{k},\omega_n)$ ⊕ continuação analítica $i\omega_n \to \omega + i\eta \to \tilde{G}_\alpha^R(\vec{k},\omega)$

" " " $i\omega_n \to \omega - i\eta \to \tilde{G}^A(\vec{k},\omega)$

$G \to \tilde{G}^R$ (292.3)




$G \to \tilde{G}^A$

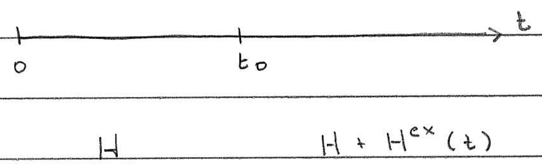
↳ ideia: determinar $G$ e, em seguida, $\tilde{G}^{R,A}$!

Resposta linear a temperatura finita.

ideia: generalizar a discussão caso $T=0$ (veja pg. 217) p/ o caso $T \neq 0$.

· resposta linear $T \neq 0$: formulação geral:

Lembrar hipótese (218.2): perturbação externa dependente do tempo atua sob sistema p/ $t \geq t_0$:




(293.1)

Eq. (220.2): p/ observável $\hat{B}_S(t)$, a resposta linear do (estado fundamental $|\psi_0\rangle$) do sistema à perturbação externa $H^{ex}(t)$:

$$\delta\langle \hat{B}(t)\rangle = \langle \psi_S(t)|\hat{B}_S(t)|\psi_S(t)\rangle - \langle \psi_0|\hat{B}_H(t)|\psi_0\rangle$$

$$= \frac{i}{\hbar}\int_{t_0}^{t} dt' \, \langle \psi_0|\left[H_H^{ext}(t') ; \hat{B}_H(t)\right]|\psi_0\rangle \qquad (293.2)$$

· considerar: $|j,N\rangle$: autoestado $H$ e op. número $\hat{N}$:

$$H|j,N\rangle = E_j(N)|j,N\rangle \quad \text{e} \quad \hat{N}|j,N\rangle = N|j,N\rangle$$

Eq. (293.2)

$$\hookrightarrow \delta\langle j,N|\hat{B}(t)|j,N\rangle = \frac{i}{\hbar}\int_{t_0}^{t} dt' \, \langle j,N|\left[H_H^{ext}(t') ; B_H(t)\right]|j,N\rangle,$$

onde: $H_H^{ext}(t)$, $\hat{B}_H(t)$ : ops. versão de Heisenberg $\quad t > t_0 \qquad$ (293.3)

$\hookrightarrow \delta\langle\hat{B}(t)\rangle = \frac{1}{Z}\sum_{j,N} e^{-\beta(E_j(N)-\mu N)}\,\delta\langle j,N|\hat{B}(t)|j,N\rangle$

$$= \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\frac{1}{Z}\,Tr\left(e^{-\beta K}[H_H^{ex}(t');\hat{B}_H(t)]\right),\ t>t_0: \qquad (294.1)$$

: generalização Eq. (293.2)

· similar Eq. (221.4), considerar:

$$H^{ex}(t) = \int d^3r\,\varphi(\vec{r},t)\,\hat{A}(\vec{r}) \to H_H^{ex}(t) = \int d^3r\,\varphi(\vec{r},t)\,\hat{A}_H(\vec{r},t) \qquad (294.2)$$

onde $\varphi(\vec{r},t)=0$ p/ $t<t_0$

$\hookrightarrow$ Eq. (294.1):

$$\delta\langle\hat{B}(\vec{r},t)\rangle = \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\frac{1}{Z}\,Tr\left(e^{-\beta K}[H_H^{ex}(t'),\hat{B}_H(\vec{r},t)]\right)$$

$$= \frac{-i}{\hbar}\int_{t_0}^{t} dt'\int d^3r'\,\frac{1}{Z}\,Tr\left(e^{-\beta K}[\hat{B}_H(\vec{r},t);\hat{A}_H(\vec{r}',t')]\right)\varphi(\vec{r}',t')$$

$$= \frac{1}{\hbar}\int_{t_0}^{t} dt'\int d^3r'\,D_{AB}^{R}(\vec{r},t;\vec{r}',t')\,\varphi(\vec{r}',t'): \qquad (294.3)$$

: veja Eq. (221.5)

onde:

$$i D_{AB}^{R}(\vec{r},t;r',t') = \frac{1}{Z}\,Tr\left(e^{-\beta K}[\hat{B}_H(\vec{r},t);\hat{A}_H(\vec{r}',t')]\right)\Theta(t-t'): \qquad (294.4)$$

: função de correlação retardada: veja Eq. (284.1)

notar Eq. (294.3): análise teoria de resposta linear
~ determinação $D^R_{AB}$!

· se $H \neq H(t) \rightarrow D^R_{AB}(\vec{r},t;\vec{r}',t') = D^R_{AB}(\vec{r},\vec{r}',t-t')$

se $[\hat{A},\hat{N}] = [\hat{B},\hat{N}] = 0$

$$\hookrightarrow \hat{A}_H(\vec{r},t) = e^{iHt/\hbar}\,\hat{A}_S(\vec{r})\,e^{-iHt/\hbar} \rightarrow e^{iKt/\hbar}\,\hat{A}_S(t)\,e^{-iKt/\hbar} \qquad (295.1)$$

· verifica-se que (via rep. de Lehmann) que a transformada de Fourier $D^R_{AB}(\vec{r},\vec{r}',\omega)$ é analítica no semi-plano superior, i.e., p/ $\mathrm{Im}\,\omega > 0$.

· similar relação entre $\mathcal{G}$ e $\bar{G}$, é interessante introduzir a função de correlação de tempo imaginário:

$$\mathcal{D}_{AB}(\vec{r},\tau;\vec{r}',\tau') = \frac{-1}{Z}\,\mathrm{Tr}\left[e^{-\beta K}\,T_\tau\left(\hat{B}_H(\vec{r},\tau)\,\hat{A}_H(\vec{r}',\tau')\right)\right] \qquad (295.2)$$

onde : $A_H(\vec{r},\tau) = e^{K\tau/\hbar}\,A_S(\vec{r})\,e^{-K\tau/\hbar}$ : comparar Eq. (222.3)

como $\mathcal{D}(\vec{r},\tau;\vec{r}',\tau') = \mathcal{D}(\vec{r},\vec{r}',\tau-\tau') \rightarrow$ transf. Fourier: $\mathcal{D}(\vec{r},\vec{r}',\nu_n)$;
via representação de Lehmann, verifica-se que:

$$\mathcal{D} \xrightarrow{\text{continuação analítica}} D^R$$

similar

$$\mathcal{G} \qquad \text{"} \qquad \bar{G}^R \quad : \text{Eq. } (292.3)$$

· próxima etapa: considerar a função de correlação densidade-densidade;

hipótese: sistema homogêneo;

Lembrar definição (200.2):

$$\hat{\rho}(\vec{r}) = \sum_{\alpha} \psi_{\alpha}^{+}(\vec{r})\, \psi_{\alpha}(\vec{r})$$

$\hookrightarrow \tilde{\rho}(\vec{r}) = \hat{\rho}(\vec{r}) - \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta K} \hat{\rho}(\vec{r})\right) = \hat{\rho}(\vec{r}) - \langle \hat{\rho}(\vec{r}) \rangle$

$\hookrightarrow$ funções de correlação densidade-densidade:

$$\mathcal{D}(\vec{r},\tau;\vec{r}',\tau') = -\frac{1}{Z} \mathrm{Tr}\left[ e^{-\beta K} T_{\tau}\left( \tilde{\rho}_H(\vec{r},\tau)\, \tilde{\rho}_H(\vec{r}',\tau') \right) \right]$$

e (296.1)

$$i D^{R}(\vec{r},\tau;\vec{r}',\tau') = \frac{1}{Z} \mathrm{Tr}\left( e^{-\beta K} \left[ \tilde{\rho}_H(\vec{r},t) ; \tilde{\rho}_H(\vec{r}',t') \right] \right) \theta(t-t') \quad :$$

: comparar Eq. (200.4)

· transformada de Fourier (248.2):

$$\mathcal{D}(\vec{r}-\vec{r}',\tau-\tau') = \frac{1}{\beta\hbar} \sum_{n\ \text{par}} \int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}\, e^{-i\nu_n(\tau-\tau')}\, \mathcal{D}(\vec{q},\nu_n)$$

notar : $\nu_n = 2n\pi/\beta\hbar$

(296.2)

$$D(\vec{r}-\vec{r}',t-t') = \int \frac{d^3q\, d\omega}{(2\pi)^4}\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}\, e^{-i\omega(t-t')}\, D(\vec{q},\omega)$$

· verifica-se que (exercício) as respectivas representações de Lehmann assumem a forma:

$$\mathcal{D}(\vec{q},\nu_n) = \hbar \int \frac{d\omega'}{2\pi} \cdot \frac{\Delta(\vec{q},\omega')}{i\nu_n - \omega'}$$

(296.3)

$$D^{R}(\vec{q},\omega) = \hbar \int \frac{d\omega'}{2\pi} \cdot \frac{\Delta(\vec{q},\omega')}{\omega - \omega' + i\eta}$$

: veja Eqs. (289.2) e (292.2)

onde:

$$\hbar\,\Delta(\vec{q},\omega) = \frac{1}{Z}\sum_{l,m} e^{-\beta K_l}(2\pi)^3\,\delta\left(\vec{q}-(\vec{p}_m-\vec{p}_l)/\hbar\right)\,*$$

$$*\,2\pi\,\delta\left(\omega-(K_m-K_l)/\hbar\right)(1-e^{-\beta\hbar\omega})\,|\langle l|\tilde{\rho}(0)|m\rangle|^2 : \qquad (297.1)$$

: veja Eq. (289.1)

· notar Eq. (296.3): polos $D^R(\vec{q},\omega)$ localizados abaixo eixo $\mathrm{Re}\,\omega$;

lembrar (223.2): " " $\sim$ excitações neutras!

· similar pg. 201, verifica-se que (exercício):

$$\mathcal{D}(\vec{r},\tau;\vec{r}',\tau') - \langle\hat{\rho}_H(\vec{r},\tau)\rangle\langle\hat{\rho}_H(\vec{r},\tau')\rangle =$$

$$= -\frac{1}{Z}\sum_{\alpha\beta} \mathrm{Tr}\left[e^{-\beta K}\,T_\tau\left(\psi^\dagger_\alpha(\vec{r},\tau)\psi_\alpha(\vec{r},\tau)\psi^\dagger_\beta(\vec{r}',\tau')\psi_\beta(\vec{r},\tau)\right)\right] \qquad (297.2)$$

e similar Eq. (261.2), temos que:

$$\mathcal{D}(\vec{r},\tau;\vec{r}',\tau') - \langle\hat{\rho}_H(\vec{r},\tau)\rangle\langle\hat{\rho}_H(\vec{r}',\tau')\rangle =$$

$$= -\sum_{\alpha\beta}\sum_{n\geq 0}\left(\frac{-1}{\hbar}\right)^n\frac{1}{n!}\int_0^{\beta\hbar} d\tau'_1\ldots d\tau'_n\,\frac{1}{Z_0}\,\mathrm{Tr}\left[e^{-\beta K_0}\,*\right.$$

$$\left.*\,T_\tau\left(V_I(\tau'_1)\ldots V_I(\tau'_n)\,\psi^\dagger_{I\alpha}(\vec{r},\tau)\psi_{I\alpha}(\vec{r}',\tau')\psi^\dagger_{I\beta}(\vec{r},\tau)\psi_{I\beta}(\vec{r}',\tau')\right)\right]$$

conectados

(297.3)

· Considerar: termo $n=0$ série (297.3):

$$(\mathrm{I}) = -\sum_{\alpha\beta} \frac{1}{Z_0} \mathrm{Tr}\left[ e^{-\beta K_0} T_\tau \left( \psi^\dagger_\alpha(\vec{r},\tau)\, \psi_\alpha(\vec{r},\tau)\, \psi^\dagger_\beta(\vec{r}',\tau')\, \psi_\beta(\vec{r}',\tau') \right) \right]$$

Eq. (260.3)

$$= -\sum_{\alpha\beta} \psi^\dagger_\alpha(\vec{r},\tau)\, \psi_\alpha(\vec{r},\tau)\, \psi^\dagger_\beta(\vec{r}',\tau')\, \psi_\beta(\vec{r}',\tau') \; +$$

$$-\langle \hat{\rho}_H(\vec{r},\tau)\rangle_0 \langle \hat{\rho}_H(\vec{r}',\tau')\rangle_0 \quad :$$

$\vec{r},\tau$ $\quad$ $\vec{r}',\tau'$ :

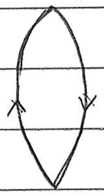
: termo ordem mais baixa (diagrama conectado) da série perturbativa de $-\langle \hat{\rho}_H(\vec{r},\tau)\rangle \langle \hat{\rho}_H(\vec{r}',\tau')\rangle$

$$\mp \sum_{\alpha\beta} \psi_\alpha(\vec{r},\tau)\, \psi^\dagger_\beta(\vec{r}',\tau')\, \psi_\beta(\vec{r}',\tau')\, \psi_\alpha(\vec{r},\tau)$$

$$\sum_{\alpha\beta} \mathcal{G}^0_{\alpha\beta}(\vec{r},\tau;\vec{r}',\tau')\, \mathcal{G}^0_{\beta\alpha}(\vec{r}',\tau';\vec{r},\tau)$$

$$(2S+1)\, \mathcal{G}^0(\vec{r},\tau;\vec{r}',\tau')\, \mathcal{G}^0(\vec{r}',\tau';\vec{r},\tau) \quad : \qquad (298.1)$$

$\vec{r},\tau$



$\vec{r}',\tau'$

de fato: série (297.3) p/ $\mathcal{D}$ formada por diagramas conectados tais que os pontos $(\vec{r},\tau)$ e $(\vec{r}',\tau')$ estão conectados por linhas internas;
diagramas conectados "do tipo produto" =
= série perturbativa de $-\langle \hat{\rho}_H(\vec{r},\tau)\rangle \langle \hat{\rho}_H(\vec{r}',\tau')\rangle$

· similar Eq. (203.3), é possível estabelecer uma relação entre $\mathcal{D}$ e a polarização total:

$$\mathcal{D}(\vec{r},\tau;\vec{r}',\tau') = \hbar\, \tilde{\pi}(\vec{r},\tau;\vec{r}',\tau') \qquad (298.2)$$

· lembrar: Eq. de Dyson permite determinar $\tilde{\pi}(\vec{q},\nu_n)$ em termos de $\pi(q,\nu_n)$: polarização própria (277.1); veja Eq. (191.4):

$$\tilde{\Pi}(\vec{q},\nu_n) = \frac{\Pi(\vec{q},\nu_n)}{1 - V(\vec{q})\,\Pi(\vec{q},\nu_n)} \qquad (299.1)$$

verifica-se que a representação de Lehmann de $\Pi(\vec{q},\nu_n)$ assume a forma:

$$\Pi(\vec{q},\nu_n) = \int \frac{d\omega'}{2\pi} \cdot \frac{\bar{\Delta}(\vec{q},\omega')}{i\nu_n - \omega'} \qquad (299.2)$$

onde $\bar{\Delta}(\vec{q},\omega) = -\bar{\Delta}(-\vec{q},-\omega) \in \mathbb{R}$

Definição:

$$F(\vec{q},z) = \int \frac{d\omega'}{2\pi} \cdot \frac{\bar{\Delta}(\vec{q},\omega')}{z - \omega'} \quad ; \; z \in \mathbb{C}$$

↳ $\Pi(\vec{q},\nu_n) = F(\vec{q},i\nu_n)$

$$\hbar\tilde{\Pi}(\vec{q},\nu_n) = \mathcal{D}(\vec{q},\nu_n) = \frac{F(\vec{q},i\nu_n)}{1 - V(\vec{q})\,F(\vec{q},i\nu_n)}$$

↳ via a continuação analítica $z \to \omega + i\eta$:

$$\hbar\tilde{\Pi}^R(\vec{q},\omega) = \mathcal{D}^R(\vec{q},\omega) = \frac{F(\vec{q},\omega+i\eta)}{1 - V(\vec{q})\,F(\vec{q},\omega+i\eta)} \quad : \qquad (299.3)$$

: comparar c/ Eq. (289.4)

Obs.: p/ aplicações do formalismo de resposta linear a temperatura finita, veja Secs. 33 e 34, Fetter.