Funções de Green - $T=0$.

Refs.: Sec. 7, Fetter and Walecka
Secs. 2.7 e 2.8, Landau
Cap. 5, Coleman
Cap. 7, AGD

ideia: • introduzir o conceito de função de Green de 1-partícula p/ um sistema de muitas partículas à temperatura $T=0$;
• há vários tipos de funções de Green;
• $\langle$ Ops. 1 corpo $\rangle$ ~ função de Green;
• espectro excitação sistema interagente ~ função de Green;
• útil p/ desenvolvimento procedimento perturbativo p/ sistema de muitas partículas.

inicial I: versão/representação de Heisenberg da M.Q.:

Lembrar representação de Schrödinger da M.Q.:

(i) $|\psi(t_0)\rangle \xrightarrow{U(t,t_0)} |\psi(t)\rangle$: evolução temporal atribuída ao estado do sistema e

(ii) $A \neq A(t)$: em geral, observáveis são estacionários exceto por dependência temporal explícita; (123.1)

onde $U(t,t_0)$: Op. evolução temporal.

• como o vetor $|\psi(t)\rangle$ é um objeto auxiliar na descrição do sistema quântico, formulações alternativas são possíveis desde que:

(i) o espectro de autovalores dos observáveis seja preservado e

(ii) o produto escalar entre autovetores $|n\rangle$ e o estado do sistema $|\psi\rangle$, i.e., $\langle n|\psi\rangle$ seja preservado: (124.1)

: essas condições podem ser satisfeitas via uma transformação unitária!

notação:

$|\psi(t)\rangle \to |\psi_S(t)\rangle$: estado do sistema na rep. Schrödinger

$A \to A_S$: observável " " "

↳ $|\psi_S(t)\rangle = U(t,t_0)|\psi_S(t_0)\rangle$

Define-se: estado do sistema $|\psi_H\rangle$ e observável $A_H(t)$ na rep. de Heisenberg da M.Q.:

· $|\psi_H\rangle \equiv U^\dagger(t,t_0)|\psi_S(t)\rangle = U^\dagger(t,t_0)U(t,t_0)|\psi_S(t_0)\rangle = |\psi_S(t_0)\rangle$

· $A_H(t) = U^\dagger(t,t_0)\, A_S\, U(t,t_0)$ (124.2)

nesse caso:

(i) estado do sistema descrito por estado estacionário $|\psi_H\rangle$

e (ii) observáveis $A_H(t)$ apresentam evolução temporal de acordo c/ eq. (de movimento) de Heisenberg.

· em particular, p/ op. de campo $\hat{\psi}_\alpha(\vec{r})$, $t_0 = 0$ e $H \neq H(t)$, temos que:

$$\hat{\psi}_{H\alpha}(\vec{r},t) = e^{iHt/\hbar}\, \hat{\psi}_{S\alpha}(\vec{r})\, e^{-iHt/\hbar} \quad : \text{veja Eq. (38.3)} \qquad (124.3)$$

notação : $\hat{\psi}_{H\alpha}(\vec{r},t) \to \psi_\alpha(\vec{r},t)$

$\hat{\psi}_{S\alpha}(\vec{r},t) \to \psi_\alpha(\vec{r})$; α : índice spin

↳ Eq. (124.3) : $\psi_\alpha(\vec{r},t) = e^{iHt/\hbar}\, \psi_\alpha(\vec{r})\, e^{-iHt/\hbar}$ (125.1)

notar :

$$i\hbar \partial_t \psi_\alpha(\vec{r},t) = i\hbar \left(\frac{iH}{\hbar}\right) \psi_\alpha(\vec{r},t) + i\hbar\, \psi_\alpha(\vec{r},t) \left(\frac{-iH}{\hbar}\right)$$

$$= -H\, \psi_\alpha(\vec{r},t) + \psi_\alpha(\vec{r},t)\, H$$

↳ $i\hbar \partial_t \psi_\alpha(\vec{r},t) = [\psi_\alpha(\vec{r},t) ; H] = e^{iHt/\hbar} [\psi_\alpha(\vec{r}), H]\, e^{-iHt/\hbar}$:

: eq. de movimento p/ $\psi_\alpha(\vec{r},t)$: veja Eq. (38.4) (125.2)

· sobre a álgebra (43.1) :

$$\underset{\uparrow \atop \mathbb{1}}{\psi_\alpha(\vec{r})}\, \psi^+_\beta(\vec{r}') \mp \psi^+_\beta(\vec{r}')\, \underset{\uparrow \atop \mathbb{1}}{\psi_\alpha(\vec{r})} = \delta_{\alpha\beta}\, \delta(\vec{r}-\vec{r}')$$

↳ $e^{iHt/\hbar}\, \psi_\alpha(\vec{r})\, e^{-iHt/\hbar}\; e^{iHt/\hbar}\, \psi^+_\beta(\vec{r})\, e^{-iHt/\hbar}$

$\pm\, e^{iHt/\hbar}\, \psi^+_\beta(\vec{r})\, e^{-iHt/\hbar}\; e^{iHt/\hbar}\, \psi_\alpha(\vec{r})\, e^{-iHt/\hbar} = \delta_{\alpha\beta}\, \delta(\vec{r}-\vec{r}')$

↳ $[\psi_\alpha(\vec{r},t) ; \psi_\beta(\vec{r}',t)]_\mp = [\psi^+_\alpha(\vec{r},t) ; \psi^+_\beta(\vec{r},t)]_\mp = 0$

e $[\psi_\alpha(\vec{r},t) ; \psi^+_\beta(\vec{r},t)]_\mp = \delta_{\alpha\beta}\, \delta(\vec{r}-\vec{r}')$: (125.3)

: importante : p/ instante de tempo t !

· inicial II: operador de ordenamento temporal T:

Definição: $T[H(t_1)H(t_2)\dots H(t_N)]$: produto cronológico operadores $H(t_1), H(t_2), \dots H(t_N)$ (126.1)

Ex.: . $T[H(t_1)H(t_2)] = \begin{cases} H(t_1)H(t_2), & \text{se } t_1 > t_2 \\ H(t_2)H(t_1), & \text{se } t_2 > t_3 \end{cases}$

· p/ $t_3 > t_1 > t_2$, temos que:

$$T[H(t_1)H(t_2)H(t_3)] = H(t_3)H(t_1)H(t_2)$$

em particular, p/ ops. de campo $\psi_\alpha(\vec{r},t)$:

$$T[\psi_\alpha(\vec{r},t)\psi^\dagger_\beta(\vec{r}',t')] = \begin{cases} \psi_\alpha(\vec{r},t)\psi^\dagger_\beta(\vec{r}',t'), & t > t' \\ \pm\psi^\dagger_\beta(\vec{r}',t')\psi_\alpha(\vec{r},t), & t' > t \end{cases} \quad (126.2)$$

onde sinal superior: bósons
" inferior: férmions

Obs.: p/ conjunto $\underline{n}$ ops. fermiônicos $\psi_\alpha(\vec{r},t)$, temos que $(-1) \to (-1)^P$, onde P = # permutações sequência original de operadores p/ sequência temporalmente ordenada.

· Definição: função de Green de 1-partícula (T = 0):

$$i\,G_{\alpha\beta}(\vec{r},t;\vec{r}',t') = \frac{\langle \psi_0 | T[\,\psi_\alpha(\vec{r},t)\,\psi^{\dagger}_\beta(\vec{r}',t')\,] | \psi_0\rangle}{\langle \psi_0 | \psi_0\rangle} \qquad (127.1)$$

$|\psi_0\rangle$: estado fundamental do sistema

hipótese: $\langle \psi_0 | \psi_0 \rangle = 1$ e $H \neq H(t)$, temos que:

$$i\,G_{\alpha\beta}(\vec{r},t;\vec{r}',t') = \langle \psi_0 | T[\,\psi_\alpha(\vec{r},t)\,\psi^{\dagger}_\beta(\vec{r}',t')\,] | \psi_0\rangle \qquad (127.2)$$

onde ops. de campo: Eq. (125.1),
α, β : índices de spin,
e $T[\ldots]$: Eq. (126.2)

· como $H \neq H(t)$, o tempo é homogêneo
↳ $G_{\alpha\beta}(\vec{r},t;\vec{r}',t') = G_{\alpha\beta}(\vec{r},\vec{r}';t-t')$;

de fato, Eqs. (125.1) e (127.2):

$$i\,G_{\alpha\beta}(\vec{r},t;\vec{r}',t') = \begin{cases} e^{iE_0(t-t')/\hbar}\,\langle \psi_0 | \psi_\alpha(\vec{r})\, e^{-iH(t-t')/\hbar}\,\psi^{\dagger}_\beta(\vec{r}') | \psi_0\rangle, & t > t' \\ \pm\, e^{-iE_0(t-t')/\hbar}\,\langle \psi_0 | \psi^{\dagger}_\beta(\vec{r}')\, e^{iH(t-t')/\hbar}\,\psi_\alpha(\vec{r}) | \psi_0\rangle, & t' > t \end{cases} \qquad (127.3)$$

· hipótese: sistema espacialmente homogêneo (e.g., líquidos e gases), temos que:

$$G_{\alpha\beta}(\vec{r},t;\vec{r}',t') = G_{\alpha\beta}(\vec{r}-\vec{r}';t-t') \qquad (127.4)$$

· hipótese: ausência campos magnéticos externos e ordenamento magnético, temos que:

$$G_{\alpha\beta}(\vec{r},t;\vec{r}',t') = \delta_{\alpha\beta}\, G_{\alpha\alpha}(\vec{r}-\vec{r}';t-t') \qquad (128.1)$$

Obs.: possível interpretação Eq. (127.2): considerar, e.g., $t > t'$; temos que:

$$i\,G_{\alpha\beta}(\vec{r},t;\vec{r}',t') = \underbrace{\langle \psi_0 | e^{iHt/\hbar}\, \psi_\alpha(\vec{r})}_{\langle \Phi'(t)|}\ \underbrace{e^{-iH(t-t')/\hbar}\, \psi^\dagger_\beta(\vec{r}')\, e^{-iHt'/\hbar} |\psi_0\rangle}_{|\Phi(t)\rangle} : \qquad (128.2)$$

: produto escalar $\langle \Phi'(t) | \Phi(t) \rangle$, onde:

$|\Phi(t)\rangle$: estado obtido a partir de $|\psi_0\rangle$ ⊕ evolução temporal ⊕ adição partícula spin β na posição $\vec{r}'$ no instante t' ⊕ evolução temporal

e $|\Phi'(t)\rangle$: " " " " " " ⊕ "
" ⊕ " " " α " "
$\vec{r}$ " " t;

Similar p/ $t' > t$.

· próxima etapa: determinação relação entre ⟨observável⟩ e $G_{\alpha\beta}(\vec{r},t;\vec{r}',t')$;

Lembrar: op. 1 corpo/partícula em termos op. de campo, veja, e.g., Eqs. (43.2) e (44.3):

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

$$\hookrightarrow \langle \hat{O}(\vec{r}) \rangle = \langle \psi_0 | \hat{O}(\vec{r}) | \psi_0 \rangle = \sum_{\alpha\beta} \langle \psi_0 | \psi^\dagger_\beta(\vec{r})\, O_{\beta\alpha}(\vec{r})\, \psi_\alpha(\vec{r}) | \psi_0 \rangle$$

$$\langle \hat{O}(\vec{r}) \rangle = \lim_{\vec{r}' \to \vec{r}} \sum_{\alpha\beta} \underbrace{\langle \Psi_0 | \Psi^{\dagger}_{\beta}(\vec{r}') \, O_{\beta\alpha}(\vec{r}) \, \Psi_{\alpha}(\vec{r}) | \Psi_0 \rangle}$$

$$O_{\beta\alpha}(\vec{r}) \underbrace{\langle \Psi_0 | \Psi^{\dagger}_{\beta}(\vec{r}') \Psi_{\alpha}(\vec{r}) | \Psi_0 \rangle}, \text{ pois } \vec{r}' \neq \vec{r}$$

$$\underbrace{\langle \Psi_0 | e^{iHt/\hbar} \Psi^{\dagger}_{\beta}(\vec{r}') e^{-iHt/\hbar} e^{iHt/\hbar} \Psi_{\alpha}(\vec{r}) e^{-iHt/\hbar} | \Psi_0 \rangle}$$

$$\langle \Psi_0 | \Psi^{\dagger}_{\beta}(\vec{r}', t) \Psi_{\alpha}(\vec{r}, t) | \Psi_0 \rangle$$

$$= \lim_{t' \to t^+} \lim_{\vec{r}' \to \vec{r}} \sum_{\alpha\beta} O_{\beta\alpha}(\vec{r}) \underbrace{\langle \Psi_0 | \Psi^{\dagger}_{\beta}(\vec{r}', t') \Psi_{\alpha}(\vec{r}, t) | \Psi_0 \rangle}_{\pm i \, G_{\alpha\beta}(\vec{r}, t; \vec{r}', t')}$$

: veja Eq. (127.3)

notar: limite é tal que $t' > t$!

$$= \pm i \lim_{t' \to t^+} \lim_{\vec{r} - \vec{r}'} \underbrace{\sum_{\alpha\beta} O_{\alpha\beta}(\vec{r}) \, G_{\alpha\beta}(\vec{r}, t; \vec{r}', t')}_{} :$$

$$= Tr\Big(O(\vec{r}) \, G(\vec{r}, t; \vec{r}', t') \Big) \qquad (129.1)$$

: valor esperado observável 1-corpo em termos de função de Green de 1 partícula!

Ex. 1: op. densidade (43.2):

$$\langle \hat{\rho}(\vec{r}) \rangle = \pm i \lim_{t' \to t^+} \lim_{\vec{r}' \to \vec{r}} \sum_{\alpha} \delta_{\alpha\beta} \, G_{\alpha\beta}(\vec{r}, t; \vec{r}', t')$$

$$= \pm i \sum_{\alpha} G_{\alpha}(\vec{r}, t; \vec{r}, t^+) \qquad (129.2)$$

Ex. 2: op. número (38.1):

$$\langle \hat{N} \rangle = \pm i \sum_{\alpha} \int d^3r \, G_{\alpha\alpha}(\vec{r}, t; \vec{r}, t^+) \qquad (129.3)$$

Ex. 3: op. densidade de spin (44.3):

$$\langle \vec{S}(\vec{r}) \rangle = \pm i \sum_{\alpha\beta} \frac{\hbar}{2} (\vec{\sigma})_{\beta\alpha} G_{\alpha\beta}(\vec{r},t;\vec{r},t^+) \tag{130.1}$$

Ex. 4: op. energia cinética (36.3):

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

$$\hookrightarrow \langle \hat{T} \rangle = \pm i \sum_{\alpha} \int d^3r \lim_{\vec{r}' \to \vec{r}} \left(-\frac{\hbar^2}{2m}\nabla^2\right) G_{\alpha\alpha}(\vec{r},t;\vec{r}',t^+) \tag{130.2}$$

· sobre o $\langle \hat{V} \rangle$: termo de interacção (37.1);
como $\hat{V}$: op. de 2 corpos → em princípio,
$V \sim$ função de Green de 2 partículas;
entretanto, verifica-se que é possível expressar $\langle \hat{V} \rangle$
em termos da função de Green de 1 partícula;

considerar: Eq. de campo (38.4) ⊕ índice spin α e $U(\vec{r})=0$;
temos que (veja pg. 130.1 p/ detalhes):

$$\left(i\hbar\partial_t - \hat{T}(\vec{r})\right)\psi_{\alpha}(\vec{r},t) =$$

$$= \sum_{\beta} \int d^3r' \, \psi^{+}_{\beta}(\vec{r}',t) \, V(\vec{r},\vec{r}') \, \psi_{\beta}(\vec{r}',t) \, \psi_{\alpha}(\vec{r},t) \tag{130.2}$$

$\hookrightarrow \langle \psi_0 | \sum_{\alpha} \int d^3r \, \psi^{+}_{\alpha}(\vec{r},t) \,*\, \text{Eq.}(130.2) \, | \psi_0 \rangle$:

R.H.S. : $\sum_{\alpha\beta} \int d^3r \, d^3r' \, \langle \psi_0 | \psi^{+}_{\alpha}(\vec{r},t) \psi^{+}_{\beta}(\vec{r}',t) V(\vec{r},\vec{r}') \,*$

$* \, \psi_{\beta}(\vec{r}',t) \psi_{\alpha}(\vec{r},t) | \psi_0 \rangle = 2\langle \hat{V} \rangle$: veja Eq. (43.3)

· Detalhes Eq. (130.2):

considerar: Eq. de movimento (125.2) e hamiltoniano (43.3)
p/ $U(\vec{r}) = 0$:

$$i\hbar\partial_t \psi_\alpha(\vec{r},t) = e^{iHt/\hbar}[\psi_\alpha(\vec{r}), H]e^{-iHt/\hbar} \qquad (130.3)$$

$$\cdot\ [\psi_\alpha(\vec{r}), \hat{T}] = \sum_\beta \int d^3r' \underbrace{[\psi_\alpha(\vec{r}) ; \psi^\dagger_\beta(\vec{r}')T(\vec{r}')\psi_\beta(\vec{r}')]}_{(I)}$$

considerando inicialmente p/ férmions ⊕ identidade:

$$[A, BC] = \{A,B\}C - B\{A,C\}, \qquad (130.4)$$

temos que:

$$(I) = \{\psi_\alpha(\vec{r}) ; \psi^\dagger_\beta(\vec{r}')\}T(\vec{r}')\psi_\beta(\vec{r}') = \delta_{\alpha\beta}\,\delta(\vec{r}-\vec{r}')T(\vec{r}')\psi_\beta(\vec{r}')$$

$$\hookrightarrow [\psi_\alpha(\vec{r}), \hat{T}] = T(\vec{r})\psi_\alpha(\vec{r}) \qquad (130.5)$$

$$\cdot\ [\psi_\alpha(\vec{r}), \hat{V}] = \frac{1}{2}\sum_{\mu\nu}\int d^3r_1 d^3r_2\, \underbrace{[\psi_\alpha(\vec{r}) ; \psi^\dagger_\mu(\vec{r}_1)\psi^\dagger_\nu(\vec{r}_2) V(\vec{r}_1,\vec{r}_2)\psi_\nu(\vec{r}_2)\psi_\mu(\vec{r}_1)]}_{(II)}$$

Lembrar identidade: $[A, BC] = [A,B]C + B[A,C]$

$$\hookrightarrow (II) = \underbrace{[\psi_\alpha(\vec{r}) ; \psi^\dagger_\mu(\vec{r}_1)\psi^\dagger_\nu(\vec{r}_2)]}\, V(\vec{r}_1,\vec{r}_2)\psi_\nu(\vec{r}_2)\psi_\mu(\vec{r}_1)$$

$$\underbrace{\{\psi_\alpha(\vec{r}) ; \psi^\dagger_\mu(\vec{r}_1)\}}_{\delta_{\alpha\mu}\,\delta(\vec{r}-\vec{r}_1)}\psi^\dagger_\nu(\vec{r}_2) - \psi^\dagger_\mu(\vec{r}_1)\underbrace{\{\psi_\alpha(\vec{r}) ; \psi_\nu(\vec{r}_2)\}}_{\delta_{\alpha\nu}\,\delta(\vec{r}-\vec{r}_2)}$$

↳ $$[\psi_\alpha(\vec r)\,;\,\hat V] = \frac{1}{2}\sum_{\nu}\int d^3 r_2\; \underset{\downarrow\,\beta}{\psi^\dagger_\nu}\,(\underset{\downarrow\,\vec r\,'}{\vec r_2})\; V(\vec r,\vec r_2)\; \underset{\downarrow\,\beta}{\psi_\nu}(\vec r_2)\;\psi_\alpha(\vec r)$$

$$-\frac{1}{2}\sum_{\mu}\int d^3 r_1\; \underset{\downarrow\,\beta}{\psi^\dagger_\mu}(\vec r_1)\; \underbrace{V(\underset{\downarrow\,\vec r\,'}{\vec r_1},\vec r)}_{=V(\vec r,\vec r\,')}\; \underbrace{\psi_\alpha(\vec r)\,\underset{\downarrow\,\beta}{\psi_\mu}(\vec r_1)}_{=-\psi_\beta(\vec r\,')\,\psi_\alpha(\vec r)}$$

$$= \sum_{\beta}\int d^3 r'\; \psi^\dagger_\beta(\vec r\,')\; V(\vec r,\vec r\,')\;\psi_\beta(\vec r\,')\;\psi_\alpha(\vec r) \qquad (130.6)$$

↳ Eqs. (130.5) ⊕ (130.6) = Eq. (130.2) !

Exercício: Verificar que Eq. (130.2) ok p/ bósons.

L.H.S. : $\sum_\alpha \int d^3r \, \langle \Psi_0 | \hat{\psi}^\dagger_\alpha(\vec{r},t) \left(i\hbar\partial_t - \hat{T}(\vec{r}) \right) \hat{\psi}_\alpha(\vec{r},t) | \Psi_0 \rangle$

$$= \pm i \sum_\alpha \int d^3r \lim_{\vec{r}' \to \vec{r}} \left(i\hbar\partial_t - \hat{T}(\vec{r}) \right) G_\alpha(\vec{r},t;\vec{r}',t^+)$$

veja Eq. (130.2)

$$\hookrightarrow \langle \hat{V} \rangle = \pm \frac{1}{2} i \sum_\alpha \int d^3r \lim_{\vec{r}' \to \vec{r}} \left(i\hbar\partial_t - \hat{T}(\vec{r}) \right) G_{\alpha\alpha}(\vec{r},t;\vec{r}',t^+) \qquad (131.1)$$

↳ energia estado fundamental em termos função de Green de 1 partícula:

$$E_0 = \langle \hat{T} + \hat{V} \rangle = \pm \frac{1}{2} i \sum_\alpha \int d^3r \lim_{\vec{r}' \to \vec{r}} \left(i\hbar\partial_t - \frac{\hbar^2 \nabla^2}{2m} \right) G_{\alpha\alpha}(\vec{r},t;\vec{r}',t^+)$$

(131.2)

· é interessante considerar a função de Green no espaço de momento e frequência;
p/ um sistema homogêneo (espaço e tempo), temos que:

$$G_{\alpha\beta}(\vec{r}-\vec{r}', t-t') = \frac{1}{V} \sum_{\vec{k}} \int \frac{d\omega}{2\pi} e^{i\vec{k}\cdot(\vec{r}-\vec{r}') - i\omega(t-t')} G_{\alpha\beta}(\vec{k},\omega)$$

(131.3)

$$\overset{\text{veja pg. 47}}{=} \int \frac{d^3k \, d\omega}{(2\pi)^4} e^{i\vec{k}\cdot(\vec{r}-\vec{r}') - i\omega(t-t')} G_{\alpha\beta}(\vec{k},\omega)$$

nesse caso, $\langle \hat{N} \rangle$: Eq. (129.3) assume a forma:

$$\langle \hat{N} \rangle = \pm i \sum_\alpha \underbrace{\int d^3r}_{V} \int \frac{d^3k \, d\omega}{(2\pi)^4} \underbrace{e^{i\omega(t^+-t)}}_{= \lim_{t' \to t^+} e^{i\omega(t'-t)} \equiv \lim_{\eta \to 0^+} e^{i\omega\eta}} G_{\alpha\alpha}(\vec{k},\omega) \qquad (131.4)$$

$\hookrightarrow \langle \hat{N} \rangle = \pm i V \sum_{\alpha} \lim_{\eta \to 0^+} \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} e^{i\omega\eta} G_{\alpha\alpha}(\vec{k},\omega)$: (132.1)

: notar fator de convergência $\eta \to 0^+$!

· similar, verifica-se que (exercício):

Eq. (130.2) : $\langle \hat{T} \rangle = \pm i V \sum_{\alpha} \lim_{\eta \to 0^+} \int \frac{d^3k\, d\omega}{(2\pi)^4} e^{i\omega\eta} \frac{\hbar^2 k^2}{2m} G_{\alpha\alpha}(\vec{k},\omega)$ (132.2)

Eq. (131.2) : $E_0 = \pm \frac{i}{2} V \sum_{\alpha} \lim_{\eta \to 0^+} \int \frac{d^3k\, d\omega}{(2\pi)^4} \left(\frac{\hbar^2 k^2}{2m} + \hbar\omega \right) e^{i\omega\eta} G_{\alpha\alpha}(\vec{k},\omega)$ (132.3)

Ex. 1: Função de Green de 1 partícula p/ férmions livres;

Lembrar hamiltoniano (45.1):

$$H = \sum_{\alpha} \int d^3r\, \psi_\alpha^\dagger(\vec{r}) \left(\frac{-\hbar^2 \nabla^2}{2m} \right) \psi_\alpha(\vec{r}) = \sum_{\alpha} \sum_{\vec{k}} \epsilon(\vec{k})\, C^\dagger_{\vec{k}\alpha} C_{\vec{k}\alpha} \quad (132.4)$$

cujo estado fundamental : Eq. (46.1):

$$|FS\rangle = \prod_{\alpha} \prod_{\substack{\vec{k} \\ k \leq k_F}} C^\dagger_{\vec{k}\alpha} |0\rangle \quad : \text{Fermi sphere} \quad (132.5)$$

nesse caso, é interessante considerarmos a expansão dos ops. de campo em termos dos ops. $C^\dagger_{\vec{k}\alpha}$ e $C_{\vec{k}\alpha}$, Eq. (42.2):

$$\psi_\alpha(\vec{r}) = \frac{1}{V^{1/2}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} C_{\vec{k}\alpha}$$

$$\hookrightarrow \psi_\alpha(\vec{r},t) = \frac{1}{V^{1/2}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} C_{\vec{k}\alpha}(t) \quad (132.5)$$

onde (verificar) : $C_{\vec{k}\alpha}(t) = C_{\vec{k}\alpha}\, e^{-i\epsilon(\vec{k})t/\hbar}$

Eq. (127.1): $i G_{\alpha\beta}(\vec{r}, t; \vec{r}', t') = \theta(t-t') \underbrace{\langle FS | \psi_\alpha(\vec{r}, t)\, \psi^\dagger_\beta(\vec{r}', t') | FS \rangle}_{(I)}$

$$- \theta(t'-t) \underbrace{\langle FS | \psi^\dagger_\beta(\vec{r}', t')\, \psi_\alpha(\vec{r}, t) | FS \rangle}_{(II)}$$

notar:

$$\cdot (I) = \frac{1}{V} \sum_{\vec{k}, \vec{p}} e^{i\vec{k}\cdot\vec{r} - i\vec{p}\cdot\vec{r}'} \underbrace{\langle FS | C_{\vec{k}\alpha}(t)\, C^\dagger_{\vec{p}\beta}(t') | FS \rangle}_{e^{-i\epsilon(\vec{k})t/\hbar}\, e^{i\epsilon(\vec{p})t'/\hbar} \underbrace{\langle FS | C_{\vec{k}\alpha} C^\dagger_{\vec{p}\beta} | FS \rangle}_{\delta_{\alpha\beta}\, \delta_{\vec{k},\vec{p}}\, \theta(k - k_F)}}$$

$$= \delta_{\alpha\beta} \frac{1}{V} \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\, e^{-i\epsilon(\vec{k})(t-t')/\hbar}\, \theta(k - k_F)$$

$$\cdot (II) = \frac{1}{V} \sum_{\vec{k}, \vec{p}} e^{-i\vec{k}\cdot\vec{r}' + i\vec{p}\cdot\vec{r}} \underbrace{\langle FS | C^\dagger_{\vec{k}\beta}(t')\, C_{\vec{p}\alpha}(t) | FS \rangle}_{e^{i\epsilon(\vec{k})t'/\hbar - i\epsilon(\vec{p})t/\hbar} \underbrace{\langle FS | C^\dagger_{\vec{k}\beta} C_{\vec{p}\alpha} | FS \rangle}_{\delta_{\alpha\beta}\, \delta_{\vec{k},\vec{p}}\, \theta(k_F - k)}}$$

$$= \delta_{\alpha\beta} \frac{1}{V} \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\, e^{-i\epsilon(\vec{k})(t-t')/\hbar}\, \theta(k_F - k)$$

$$\hookrightarrow i G_{\alpha\alpha}(\vec{r}-\vec{r}'; t-t') = \frac{1}{V} \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\, e^{-i\epsilon(\vec{k})(t-t')/\hbar} \,*$$

$$* \Big(\theta(t-t')\,\theta(k-k_F) - \theta(t'-t)\,\theta(k_F-k) \Big) \therefore \qquad (133.1)$$

$\therefore$ comparar c/ hipótese (127.4) !

· Eq. (131.3) pode ser escrita como:

$$G_{\alpha\beta}(\vec{r}-\vec{r}', t-t') = \frac{1}{V}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} \underbrace{\int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} G_{\alpha\beta}(\vec{k},\omega)}_{\equiv G_{\alpha\beta}(\vec{k}, t-t')} \qquad (134.1)$$

↳ Eqs. (133.1) e (134.1):

$$i\, G_{\alpha\alpha}(\vec{k}, t-t') = e^{-i\epsilon(\vec{k})(t-t')/\hbar}\, \theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)) \qquad (134.2)$$

$$\hookrightarrow i\, G_{\alpha\alpha}(\vec{k},\omega) = \int d(t-t')\, e^{i\omega(t-t')}\, i\, G_{\alpha\beta}(\vec{k}, t-t')$$

$$= \int dt\, e^{i(\omega-\epsilon(\vec{k})/\hbar)t} (\theta(t)\theta(k-k_F) - \theta(-t)\theta(k_F-k))$$

$$= \theta(k-k_F)\underbrace{\int_0^{\infty} dt\, e^{i(\omega-\epsilon(\vec{k})/\hbar)t-\eta t}}_{\frac{-1}{i(\omega-\epsilon(\vec{k})/\hbar-\eta}} - \theta(k_F-k)\underbrace{\int_{-\infty}^{0} dt\, e^{i(\omega-\epsilon(\vec{k})/\hbar)t+\eta t}}_{\frac{1}{i(\omega-\epsilon(\vec{k})/\hbar)+\eta}}$$

notar: é necessário introduzir o fator de convergência $\eta > 0$!

$$\hookrightarrow \frac{1}{\hbar} G_{\alpha\alpha}(\vec{k},\omega) = \underbrace{\frac{\theta(k-k_F)}{\hbar\omega - \epsilon(\vec{k}) + i\eta}}_{\text{partícula}} + \underbrace{\frac{\theta(k_F-k)}{\hbar\omega-\epsilon(\vec{k})-i\eta}}_{\text{buraco}}$$

notar polos: partícula buraco : veja pg. 144

(134.3)

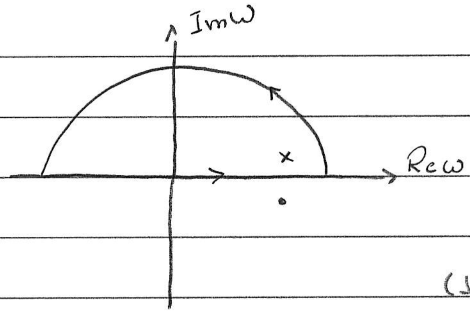
$$\text{ou } G_{\alpha\alpha}(\vec{k},\omega) = \frac{1}{\hbar\omega - \epsilon(\vec{k}) + i\eta\, \mathrm{sgn}(k-k_F)}\,\hbar$$

· notar Eqs. (132.1) e (134.3):

$$\langle \hat{N} \rangle = -iV \sum_{\alpha} \lim_{\eta' \to 0^+} \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} e^{i\omega\eta'} G_{\alpha\alpha}(\vec{k},\omega)$$

$$= -\frac{2iV}{8\pi^3} \cdot 4\pi \int_0^{\infty} k^2 dk \left(\theta(k-k_F) \underbrace{\int \frac{d\omega}{2\pi} \cdot \frac{e^{i\omega\eta'}}{\omega - \epsilon(k) + i\eta}}_{(I)} + \theta(k_F - k) \underbrace{\int \frac{d\omega}{2\pi} \cdot \frac{e^{i\omega\eta'}}{\omega - \epsilon(k) - i\eta}}_{(II)} \right) \qquad (135.1)$$

as integrais (I) e (II) podem ser determinadas por resíduos; como $\eta' \to 0^+$, temos que:



$(I) = 0$

$$(II) = \frac{1}{2\pi} \cdot 2\pi i \cdot \underset{\uparrow}{(+1)} \cdot e^{i\epsilon(k)\eta'} \xrightarrow[\eta' \to 0^+]{} i \qquad (135.2)$$

counterclockwise

x : $\epsilon(k) + i\eta$

• : $\epsilon(k) - i\eta$; $\vec{k}$ fixo

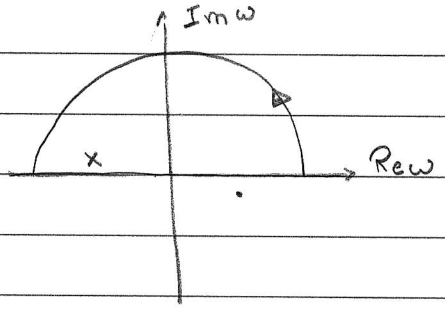
↳ $N = \langle \hat{N} \rangle = -\frac{2iV}{8\pi^3} \cdot 4\pi \cdot (i) \int_0^{k_F} k^2 dk = \frac{V k_F^3}{3\pi}$: Eq. (47.1)!

Obs.: É interessante considerar o gás de férmions no ensemble gran-canônico; nesse caso, p/ a rep. de Heisenberg dos ops. fermiônicos, é necessário considerar:

$$\hat{H} \to \hat{K} = \hat{H} - \mu \hat{N} \quad \to \epsilon(\hat{k}) = \frac{\hbar^2 k^2}{2m} - \mu$$

p/ o gás de férmions a $T = 0$, $\mu = \epsilon_F$

↳ Fig (135.1) assume a forma:



: Vejo Fig. 5.4, Coleman

(136.1)

pois: x : $\epsilon(k) + i\eta$, $\epsilon(k) < 0$ p/ $k < k_F$: buraco

• : $\epsilon(k) - i\eta$, $\epsilon(k) > 0$ p/ $k > k_F$: partícula

Exercício: mostrar que Eqs. (132.2) e (134.3) -> Eq. (48.1)

Ex. 2: Função de Green p/ fônons:

Lembrar hamiltoniano (104.3):

$$H = \sum_{s} \sum_{\vec{q} \in BZ} \hbar \omega_s(\vec{q}) \left(a^{\dagger}_{\vec{q}s} a_{\vec{q}s} + 1/2 \right) \qquad (137.1)$$

cujo estado fundamental $|0\rangle$ = vácuo bosons $\underline{a}$: $a_{\vec{q}s}|0\rangle = 0$.

nesse caso, Eq. (105.1) → definição op. de campo:

$$\phi_s(\vec{r},t) = \frac{1}{V^{1/2}} \sum_{\vec{q}} C^s_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}} \left(a_{\vec{q}s}\, e^{-i\omega_s(\vec{q})t} + a^{\dagger}_{-\vec{q}s}\, e^{+i\omega_s(\vec{q})t} \right)$$

(137.2)

$$\text{onde } C^s_{\vec{q}} = \sqrt{\frac{\hbar}{2m\omega_s(\vec{q})}} \quad ; \quad C^s_{-\vec{q}} = C^s_{\vec{q}}$$

como (137.1) descreve sistema de fônons não interagentes, podemos omitir o índice $\underline{s}$ e considerar:

$$\phi(\vec{r},t) = \frac{1}{V^{1/2}} \sum_{\vec{q}} C_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}} \left(a_{\vec{q}}\, e^{-i\omega_{\vec{q}}t} + a^{\dagger}_{-\vec{q}}\, e^{i\omega_{\vec{q}}t} \right) \qquad (137.2)$$

↳ Definição: função de Green p/ fônons:

$$i D(\vec{r},t;\vec{r}',t') = \langle 0 | T\left(\phi(\vec{r},t)\, \phi(\vec{r}',t') \right) | 0 \rangle \qquad (137.3)$$

p/ o sistema de fônons descrito pelo hamiltoniano (137.1) temos que:

$$i D^{(0)}(\vec{r},t;\vec{r}',t') = \Theta(t-t') \langle 0 | \phi(\vec{r},t)\, \phi(\vec{r}',t') | 0 \rangle$$

(137.4)

$$+ \Theta(t'-t) \langle 0 | \phi(\vec{r}',t')\, \phi(\vec{r},t) | 0 \rangle$$

temos que:

$$\langle 0|\phi(\vec{r},t)\,\phi(\vec{r}',t')|0\rangle = \frac{1}{V}\sum_{\vec{k}\vec{q}} C_{\vec{k}} C_{\vec{q}}\, e^{i(\vec{k}\cdot\vec{r}+\vec{q}\cdot\vec{r}')} +$$

$$+\underbrace{\langle 0|\left(a_{\vec{k}}e^{-i\omega_{\vec{k}}t}+a^{\dagger}_{-\vec{k}}e^{i\omega_{\vec{k}}t}\right)\left(a_{\vec{q}}e^{-i\omega_{\vec{q}}t'}+a^{\dagger}_{-\vec{q}}e^{i\omega_{\vec{q}}t'}\right)|0\rangle}$$

$$= e^{-i\omega_{\vec{k}}t+i\omega_{\vec{q}}t'}\underbrace{\langle 0|a_{\vec{k}}a^{\dagger}_{-\vec{q}}|0\rangle}$$

$$= \delta_{\vec{k},-\vec{q}} + \langle 0|a^{\dagger}_{-\vec{q}}a_{\vec{k}}|0\rangle = \delta_{\vec{k},-\vec{q}}$$

$$= \frac{1}{V}\sum_{\vec{k}} C^2_{\vec{k}}\, e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\, e^{-i\omega_{\vec{k}}(t-t')}$$

similar p/ segundo termo (137.4)

$$\hookrightarrow iD^{(0)}(\vec{r}-\vec{r}',t-t') = \frac{1}{V}\sum_{\vec{k}} C^2_{\vec{k}}\Big(e^{i\vec{k}\cdot(\vec{r}-\vec{r}')-i\omega_{\vec{k}}(t-t')}\,\theta(t-t')$$

$$+\,e^{-i\vec{k}\cdot(\vec{r}-\vec{r}')+i\omega_{\vec{k}}(t-t')}\,\theta(t'-t)\Big) \tag{138.1}$$

como: $D^{(0)}(\vec{q},\omega) = \int d^3r\,dt\; e^{-i\vec{q}\cdot\vec{r}+i\omega t}\,D^{(0)}(\vec{r},t)$: veja Eq. (131.3),

temos que:

$$iD^{(0)}(\vec{q},\omega) = \frac{1}{V}\sum_{\vec{k}} C^2_{\vec{k}}\Bigg(\underbrace{\int d^3r\, e^{-i(\vec{q}-\vec{k})\cdot\vec{r}}}_{V\delta_{\vec{q},\vec{k}}}\;\underbrace{\int dt\, e^{i(\omega-\omega_{\vec{k}})t}\,\theta(t)}_{(\mathrm{I})}$$

$$+\underbrace{\int d^3r\, e^{-i(\vec{q}+\vec{k})\cdot\vec{r}}}_{V\delta_{\vec{q},-\vec{k}}}\;\underbrace{\int dt\, e^{i(\omega+\omega_{\vec{k}})t}\,\theta(-t)}_{(\mathrm{II})}\Bigg)$$

como $(I) = \int_0^{\infty} dt\, e^{i(\omega - \omega_{\vec{k}})t - \eta t} = \dfrac{-1}{i(\omega - \omega_{\vec{k}}) - \eta}$; $\eta > 0$

e $(II) = \int_{-\infty}^{0} dt\, e^{i(\omega + \omega_{\vec{k}})t + \eta t} = \dfrac{1}{i(\omega + \omega_{\vec{k}}) + \eta}$

$$\hookrightarrow D^{(0)}(\vec{q},\omega) = C_{\vec{q}}^2 \left(\underbrace{\frac{1}{\omega - \omega_{\vec{q}} + i\eta}}_{\text{emissão}} - \underbrace{\frac{1}{\omega + \omega_{\vec{q}} - i\eta}}_{\text{absorção fônon}} \right) \qquad (139.1)$$

possível
interpretação:

ou $$D^{(0)}(\vec{q},\omega) = C_{\vec{q}}^2 \cdot \frac{2\omega_{\vec{q}}}{\omega^2 - (\omega_{\vec{q}} - i\eta)^2} \qquad (139.2)$$

Obs.: sobre definição $C_{\vec{q}}$:

$C_{\vec{q}} = 1$: Eq. (2.73), Mahan

$C_{\vec{q}} = \sqrt{\dfrac{\hbar}{2m\omega_{\vec{q}}}}$: Eq. (5.88), Coleman

$C_{\vec{q}} = \sqrt{\dfrac{\hbar\omega_{\vec{q}}}{2}}$: Eqs. (45.14) e (46.6), Fetter.

Representação de Lehmann.

ideia: determinação propriedades da função de Green;

importante: vamos considerar apenas férmions a $T=0$;

p/ bósons, é necessário considerar a formação do BEC a $T=0$.

Eq. (127.2): $$i G_{\alpha\beta}(\vec{r},t;\vec{r}',t') = \theta(t-t')\langle\psi_0|\hat{\psi}_\alpha(\vec{r},t)\underset{\uparrow \hat{1}}{\,}\hat{\psi}^\dagger_\beta(\vec{r}',t')|\psi_0\rangle$$

$$-\theta(t'-t)\langle\psi_0|\hat{\psi}^\dagger_\beta(\vec{r}',t')\underset{\uparrow}{\,}\hat{\psi}_\alpha(\vec{r},t)|\psi_0\rangle = (I)$$

$$\hat{1} = \sum_n |\psi_n\rangle\langle\psi_n|$$

onde: $|\psi_n\rangle$: autoestados $\hat{H} = \hat{T} + \hat{V}$

como $\hat{\psi}_\alpha(\vec{r},t) = e^{iHt/\hbar}\,\hat{\psi}_\alpha(\vec{r})\,e^{-iHt/\hbar}$: Eq. (125.1), temos que

$$(I) = \sum_n \theta(t-t')\,e^{-i(E_n-E_0)(t-t')/\hbar}\langle\psi_0|\hat{\psi}_\alpha(\vec{r})|\psi_n\rangle\langle\psi_n|\hat{\psi}^\dagger_\beta(\vec{r}')|\psi_0\rangle$$

$$-\theta(t'-t)\,e^{+i(E_n-E_0)(t-t')/\hbar}\langle\psi_0|\hat{\psi}^\dagger_\beta(\vec{r}')|\psi_n\rangle\langle\psi_n|\hat{\psi}_\alpha(\vec{r})|\psi_0\rangle$$

(140.1)

onde E_0: energia estado fundamental $|\psi_0\rangle$

- Lembrar: Op. número (38.1): $\hat{N} = \sum_\alpha \int d^3r\, \hat{\psi}^\dagger_\alpha(\vec{r})\,\hat{\psi}_\alpha(\vec{r})$

$$\hookrightarrow [\hat{N},\hat{\psi}_\alpha(\vec{r})] = \sum_\beta \int d^3r'\, \underbrace{[\hat{\psi}^\dagger_\beta(\vec{r}')\hat{\psi}_\beta(\vec{r}');\hat{\psi}_\alpha(\vec{r})]} = -\hat{\psi}_\alpha(\vec{r})$$

$$= -\underbrace{\{\hat{\psi}^\dagger_\beta(\vec{r}');\hat{\psi}_\alpha(\vec{r})\}}_{\delta_{\alpha\beta}\,\delta(\vec{r}-\vec{r}')}\hat{\psi}_\beta(\vec{r}')$$

$$\hookrightarrow \left(\hat{N}\hat{\psi}_\alpha(\vec{r}) - \hat{\psi}_\alpha(\vec{r})\hat{N}\right)|\psi_0\rangle = -\hat{\psi}_\alpha(\vec{r})|\psi_0\rangle$$

$$\hookrightarrow \hat{N}\left(\hat{\psi}_\alpha(\vec{r})|\psi_0\rangle\right) = (N-1)\left(\hat{\psi}_\alpha(\vec{r})|\psi_0\rangle\right) \dashrightarrow \hat{\psi}_\alpha(\vec{r})|\psi_0\rangle$$: estado c/ $(N-1)$ partículas

↳ se $\langle \psi_n | \hat{\psi}_\alpha(\vec{r}) | \psi_0 \rangle \neq 0 \rightarrow |\psi_n\rangle$: autoestado H c/ (N-1) partículas!

similar (verificar) : se $\langle \psi_n | \hat{\psi}^+_\beta(\vec{r}) | \psi_0 \rangle \neq 0 \rightarrow |\psi_n\rangle$: autoestado H c/ (N+1) partículas!

· até o momento, consideramos apenas que $H \neq H(t)$;
⊕ hipótese : sistema apresenta invariância translacional
↳ $[H, \vec{P}] = 0$, onde

$$\vec{P} = \sum_\alpha \int d^3r \, \hat{\psi}^+_\alpha(\vec{r}) (-i\hbar\vec{\nabla}) \psi_\alpha(\vec{r}) \quad (141.1)$$

: momento linear total do sistema : veja Eqs. (9.1) e (36.3)

verifica-se que (exercício):

$$-i\hbar\vec{\nabla}\hat{\psi}_\alpha(\vec{r}) = [\psi_\alpha(\vec{r}), \vec{P}] \rightarrow \hat{\psi}_\alpha(\vec{r}) = e^{-i\vec{P}\cdot\vec{r}/\hbar} \hat{\psi}_\alpha(\vec{r}=0) e^{+i\vec{P}\cdot\vec{r}/\hbar} :$$

: similar Eqs. (125.1) e (125.2)!

· notar Eq. (140.1):

$$\cdot \langle \psi_0 | \hat{\psi}_\alpha(\vec{r}) | \psi_n \rangle = \langle \psi_0 | e^{-i\vec{P}\cdot\vec{r}/\hbar} \hat{\psi}_\alpha(0) e^{i\vec{P}\cdot\vec{r}/\hbar} | \psi_n \rangle =$$

$$= e^{i\vec{P}_n\cdot\vec{r}/\hbar} \langle \psi_0 | \hat{\psi}_\alpha(0) | \psi_n \rangle \; ; \quad \vec{P}|\psi_0\rangle = 0$$

e $\vec{P}|\psi_n\rangle = \vec{P}_n|\psi_n\rangle$:

: lembrar que $[H, \vec{P}] = 0$

↳ Eq. (140.1) :

$i G_{\alpha\beta}(\vec{r}-\vec{r}', t-t') =$

$$= \sum_n \Theta(t-t')\, e^{-i(E_n-E_0)(t-t')/\hbar}\, e^{i\vec{p}_n(\vec{r}-\vec{r}')} \, *$$
$$* \langle \psi_0 | \hat{\psi}_\alpha(0) | \psi_n \rangle \langle \psi_n | \hat{\psi}^+_\beta(0) | \psi_0 \rangle$$

$$- \Theta(t'-t)\, e^{+i(E_n-E_0)(t-t')/\hbar}\, e^{-i\vec{p}_n\cdot(\vec{r}-\vec{r}')} \, *$$
$$* \langle \psi_0 | \hat{\psi}^+_\beta(0) | \psi_n \rangle \langle \psi_n | \hat{\psi}_\alpha(0) | \psi_0 \rangle \qquad (142.1)$$

como Eq. (131.3)

$$\hookrightarrow G_{\alpha\beta}(\vec{k},\omega) = \int d^3r\, dt\, e^{-i\vec{k}\cdot\vec{r}+i\omega t}\, G_{\alpha\beta}(\vec{r},t) \qquad (142.2)$$

$$\text{e} \int dt\, e^{-i(E_n-E_0-\omega)t}\,\Theta(t) = \underbrace{\int_0^\infty dt\, e^{-i(E_n-E_0-\omega)t-\eta t}}$$
$$= \frac{-1}{-i(E_n-E_0-\omega)-\eta} \quad ; \eta > 0$$

$$\text{e} \int dt\, e^{i(E_n-E_0+\omega)t}\,\Theta(-t) = \underbrace{\int_{-\infty}^0 dt\, e^{i(E_n-E_0+\omega)t+\eta t}}$$
$$= \frac{1}{i(E_n-E_0+\omega)+\eta} \quad ; \eta > 0$$

$$\text{e} \int d^3r\, \exp\left(-i(\vec{k} \mp \vec{p}_n/\hbar)\right) = V\,\delta_{\vec{k},\pm\vec{p}_n/\hbar}$$

$$\hookrightarrow G_{\alpha\beta}(\vec{k},\omega) = V \sum_n \frac{\langle \psi_0 | \hat{\psi}_\alpha(0) | \psi_n \rangle \langle \psi_n | \hat{\psi}^+_\beta(0) | \psi_0 \rangle}{\omega - (E_n-E_0)/\hbar + i\eta}\,\delta_{\vec{k},\vec{p}_n/\hbar}$$
$$+ \frac{\langle \psi_0 | \hat{\psi}^+_\beta(0) | \psi_n \rangle \langle \psi_n | \psi_\alpha(0) | \psi_0 \rangle}{\omega + (E_n-E_0)/\hbar - i\eta}\,\delta_{\vec{k},-\vec{p}_n/\hbar}$$

(142.3)

Eq. (142.3) : indica dependência explícita $G_{\alpha\beta}(\vec{k},\omega)$ c/ a frequência ω !

Obs. 1: a restrição $\delta_{\vec{k};\pm\vec{p}_n/\hbar}$ sob o momento dos estados intermediários $|\Psi_n\rangle$ pode ser indicada através da notação : $|\Psi_n\rangle \to |n,\pm\vec{k}\rangle$

Obs. 2 : vimos que os estados intermediários $|\Psi_n\rangle$ são estados c/ $(N\pm1)$ partículas;

p/ o primeiro termo Eq. (142.3), temos que $|\Psi_n\rangle$: $N+1$ partículas;

↳ $E_n - E_0 = E_n(N+1) - E_0(N) =$

$$= \underbrace{\left(E_n(N+1) - E_0(N+1)\right)}_{\equiv \varepsilon_n(N+1) > 0} + \underbrace{\left(E_0(N+1) - E_0(N)\right)}_{\mu(N+1)}$$

: energia excitação sistema N+1 partículas

$\mu(N+1)$: potencial químico (pois V = cte)

similar p/ o segundo termo Eq. (142.3):

$E_n - E_0 = E_n(N-1) - E_0(N) =$

$$= \underbrace{\left(E_n(N-1) - E_0(N-1)\right)}_{\varepsilon_n(N-1) > 0} + \underbrace{\left(E_0(N) - E_0(N-1)\right)}_{\mu(N)}$$

↳ $$G_{\alpha\beta}(\vec{k},\omega) = \hbar V \sum_n \frac{\langle\Psi_0|\hat{\Psi}_\alpha(0)|n,\vec{k}\rangle\langle n,\vec{k}|\hat{\Psi}_\beta^\dagger(0)|\Psi_0\rangle}{\hbar\omega - \mu - \varepsilon_{n,\vec{k}}(N+1) + i\eta} \tag{143.1}$$

$$+ \frac{\langle\Psi_0|\hat{\Psi}^\dagger_\beta(0)|n,-\vec{k}\rangle\langle n,-\vec{k}|\hat{\Psi}_\alpha(0)|\Psi_0\rangle}{\hbar\omega - \mu + \varepsilon_{n,-\vec{k}}(N-1) - i\eta}$$

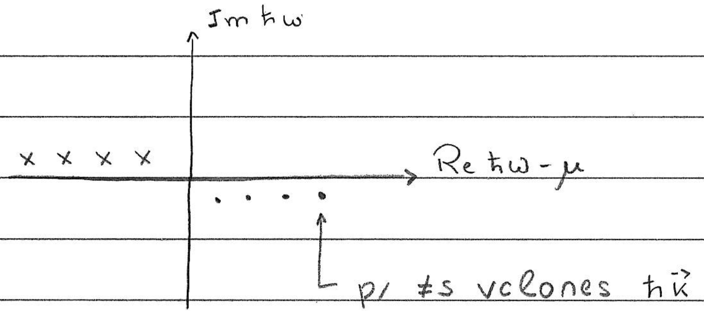
Eq. (143.1): representação de Lehmann p/ a função de Green!

· novamente: Eq. (143.1) indica dependência $G_{\alpha\beta}(\vec{k},\omega)$ em termos frequência ω;

↳ no plano $Re\,\omega - Im\,\omega$, $G_{\alpha\beta}(\vec{k},\omega)$ apresenta polos de ordem 1 = = energias excitação sistema interagente c/ momento $\hbar\vec{k}$:

1º termo: $\hbar\omega - \mu = \varepsilon_{n,\vec{k}}(N+1) - i\eta$: partícula : ·

2º termo: $\hbar\omega - \mu = -\varepsilon_{n,\vec{k}}(N-1) + i\eta$: buraco : x



(144.1)

Ex.: Eq. (143.1) p/ férmions livres;

considerando Eq. (132.5), temos que:

$$\cdot \langle \Psi_0 | \hat{\Psi}_\alpha(0) | n,\vec{k} \rangle \langle n,\vec{k} | \hat{\Psi}^\dagger_\beta(0) | \Psi_0 \rangle =$$

$$= \frac{1}{V} \sum_{\vec{p},\vec{q}} \underbrace{\langle FS | C_{\vec{p}\alpha} | n,\vec{k} \rangle \langle n,\vec{k} | C^\dagger_{\vec{q}\beta} | FS \rangle}_{\delta_{\vec{p},\vec{k}}\,\delta_{\vec{q},\vec{k}}\,\delta_{\alpha\beta}\,\Theta(k-k_F)} = \frac{1}{V}\,\delta_{\alpha\beta}\,\Theta(k-k_F)$$

similar: $\langle \Psi_0 | \hat{\Psi}^\dagger_\beta(0) | n,-\vec{k} \rangle \langle n,-\vec{k} | \Psi_\alpha(0) | \Psi_0 \rangle = \frac{1}{V}\,\delta_{\alpha\beta}\,\Theta(k_F-k)$

$\cdot\ \epsilon_{n,\vec{k}}(N+1) = E_{\vec{k}}(N+1) - E_0(N+1) = \dfrac{\hbar^2 k^2}{2m} - \dfrac{\hbar^2 k_F^2}{2m} = \epsilon(\vec{k}) - \epsilon_F > 0 \quad (i)$

$\epsilon_{n,-\vec{k}}(N-1) = E_{-\vec{k}}(N-1) - E_0(N-1) \rightarrow \dfrac{\hbar^2 k_F^2}{2m} - \dfrac{\hbar^2 k^2}{2m} = \epsilon_F - \epsilon(\vec{k}) > 0 \quad (ii)$

lembrar: (i) : $k > k_F$ e (ii) : $k < k_F$

↳ $\hbar\omega - \mu - \epsilon_{n,\vec{k}}(N+1) + i\eta = \hbar\omega - \epsilon_F - (\epsilon(\vec{k}) - \epsilon_F) + i\eta$

$= \hbar\omega - \epsilon(\vec{k}) + i\eta$

$\hbar\omega - \mu + \epsilon_{n,-\vec{k}}(N-1) - i\eta = \hbar\omega - \epsilon_F + (\epsilon_F - \epsilon(\vec{k})) - i\eta$

$= \hbar\omega - \epsilon(\vec{k}) - i\eta$:

: OK c/ Eq. (134.3)

· hipótese (128.1) : $G_{\alpha\beta}(\vec{k},\omega) = \delta_{\alpha\beta}\, G_{\alpha\alpha}(\vec{k},\omega)$;

nesse caso:

$\langle \Psi_0 | \hat{\Psi}_\alpha(0) | n,\vec{k}\rangle\langle n,\vec{k} | \hat{\Psi}^\dagger_\beta(0) | \Psi_0\rangle \rightarrow |\langle \Psi_n | \hat{\Psi}^\dagger_\alpha(0) | \Psi_0\rangle|^2 \geq 0$

e $\langle \Psi_0 | \hat{\Psi}^\dagger_\beta(0) | n,-\vec{k}\rangle\langle n,-\vec{k} | \hat{\Psi}_\alpha(0) | \Psi_0\rangle \rightarrow |\langle \Psi_n | \hat{\Psi}_\alpha(0) | \Psi_0\rangle|^2 \geq 0$

é interessante introduzir as densidades espectrais:

$$A(\vec{k},\omega) = V \sum_n |\langle n,\vec{k} | \hat{\Psi}^\dagger_\alpha(0) | \Psi_0\rangle|^2\, \delta(\omega - \epsilon_{n,\vec{k}}/\hbar)$$

(145.1)

$$\text{e}\quad B(\vec{k},\omega) = V \sum_n |\langle n,-\vec{k} | \hat{\Psi}_\alpha(0) | \Psi_0\rangle|^2\, \delta(\omega - \epsilon_{n,-\vec{k}}/\hbar)$$

como $\epsilon_{n,\vec{k}}$ e $\epsilon_{n,-\vec{k}} \geq 0 \rightarrow A(\vec{k},\omega)$ e $B(\vec{k},\omega) \neq 0$, se $\omega \geq 0$

↳ Eq. (143.1) assume a forma:

$$G_{\alpha\alpha}(\vec{k},\omega) = \int_0^\infty d\omega' \left(\frac{A(\vec{k},\omega')}{\omega - \mu/\hbar - \omega' + i\eta} + \frac{B(\vec{k},\omega')}{\omega - \mu/\hbar + \omega' - i\eta} \right) \qquad (146.1)$$

Lembrar identidade: $\dfrac{1}{\omega \pm i\eta} = P\dfrac{1}{\omega} \mp i\pi\delta(\omega)$; $\omega \in \mathbb{R}$

onde P: parte principal da integral, i.e.:

$$P\int_{x_1}^{x_2} dx \frac{f(x)}{x - x_0} = \lim_{\epsilon \to 0} \left(\int_{x_1}^{x_0-\epsilon} dx \frac{f(x)}{x-x_0} + \int_{x_0+\epsilon}^{x_2} dx \frac{f(x)}{x - x_0} \right) ; \qquad (146.2)$$

c/ $x_1 < x_0 < x_2$;

temos que:

$$\mathrm{Re}\, G_{\alpha\alpha}(\vec{k},\omega) = P\int_0^\infty d\omega' \left(\frac{A(\vec{k},\omega')}{\omega - \mu/\hbar - \omega'} + \frac{B(\vec{k},\omega')}{\omega - \mu/\hbar + \omega'} \right)$$

(146.3)

$$\text{e} \quad \mathrm{Im}\, G_{\alpha\alpha}(\vec{k},\omega) = \begin{cases} -\pi A(\vec{k}, \omega - \mu/\hbar) , & \text{se } \omega - \mu/\hbar \geq 0 \\ +\pi B(\vec{k}, \mu/\hbar - \omega) , & \text{se } \omega - \mu/\hbar \leq 0 \end{cases}$$

notar Eq. (146.3) : como $A(\vec{k},\omega)$ e $B(\vec{k},\omega) \geq 0 \to \mathrm{sgn}(\mathrm{Im}\, G_{\alpha\alpha}(\vec{k},\omega))$ é modificado p/ $\hbar\omega = \mu$!

· Eq. (146.3) $\to$ determinar relação entre $\mathrm{Re}\, G_{\alpha\alpha}(\vec{k},\omega)$ e $\mathrm{Im}\, G_{\alpha\alpha}(\vec{k},\omega)$; notar:

$$\cdot \int_0^\infty d\omega'' \frac{A(\vec{k},\omega'')}{\omega - \mu/\hbar - \omega''} = \int_{\mu/\hbar}^\infty d\omega' \frac{A(\vec{k},\omega' - \mu/\hbar)}{\omega - \omega'} = -\frac{1}{\pi}\int_{\mu/\hbar}^\infty d\omega' \frac{\mathrm{Im}\, G_{\alpha\alpha}(\vec{k},\omega')}{\omega - \omega'}$$

$\omega'' = \omega' - \mu/\hbar$

$$= \frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega' \frac{\mathrm{Im}\, G_{\alpha\alpha}(\vec{k},\omega')}{\omega' - \omega}\, \Theta(\omega' - \mu/\hbar)\, \mathrm{sgn}(\omega' - \mu/\hbar)$$

$$\int_0^{\infty} d\omega'' \frac{B(\vec{k},\omega'')}{\omega-\mu/\hbar+\omega''} = \int_{-\infty}^{\mu/\hbar} d\omega' \frac{B(\vec{k},\mu/\hbar-\omega')}{\omega-\omega'} = \frac{-1}{\pi}\int_{-\infty}^{\mu/\hbar} d\omega' \frac{\operatorname{Im} G_{\alpha\alpha}(\vec{k},\omega')}{\omega'-\omega}$$

$\omega'' = -\omega' + \mu/\hbar$

$$= \frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega' \frac{\operatorname{Im} G_{\alpha\alpha}(\vec{k},\omega')}{\omega'-\omega}\,\theta(\mu/\hbar-\omega')\,\operatorname{sgn}(\omega'-\mu/\hbar)$$

$$\hookrightarrow \operatorname{Re} G_{\alpha\alpha}(\vec{k},\omega) = \frac{1}{\pi} P\int_{-\infty}^{+\infty} d\omega' \frac{\operatorname{Im} G_{\alpha\alpha}(\vec{k},\omega')}{\omega'-\omega}\operatorname{sgn}(\omega'-\mu/\hbar) : \qquad (147.1)$$

: relação entre partes real e imaginária $G_{\alpha\alpha}(\vec{k},\omega)$!

· a representação de Lehmann (146.1) p/ a função de Green
-> determinação propriedades analíticas

(i) comportamento assintótico $\omega \to +\infty$;

$$\text{Eq. (146.1)} \to G_{\alpha\alpha}(\vec{k},\omega) \sim \frac{1}{\omega}\underbrace{\int_0^{\infty} d\omega' \left(A(\vec{k},\omega') + B(\vec{k},\omega')\right)}_{=1 \ :\ \text{veja pg. 147.1}}$$

$$\hookrightarrow G_{\alpha\alpha}(\vec{k},\omega) \xrightarrow[\omega\to+\infty]{} \frac{1}{\omega} \qquad (147.1)$$

(ii) comportamento $G_{\alpha\alpha}(\vec{k},\omega)$ no plano ω-complexo;

Eq. (146.1) -> $G_{\alpha\alpha}(\vec{k},\omega)$ apresenta polos de ordem 1 acima e abaixo eixo $\operatorname{Re}\omega$ -> G não é uma função analítica no plano ω-complexo;

$\hookrightarrow$ é interessante introduzir:

$G^R(\vec{k},\omega)$: analítica semi-plano superior : retardada

e $G^A(\vec{k},\omega)$: " " " inferior : avançada

· Detalhes Eq. (147.1),

temos que:

$$\int_0^{\infty} d\omega' \, A(\vec{k},\omega') = v \sum_n \int_0^{\infty} d\omega' |\langle n,\vec{k}|\, \hat{\psi}^{+}_{\alpha}(0) |\psi_0\rangle|^2 \, \delta(\omega' - E_{n,\vec{k}}/\hbar)$$

$$= v \sum_n \langle \psi_0 | \hat{\psi}_{\alpha}(0) | \psi_n \rangle \langle \psi_n | \hat{\psi}^{+}_{\alpha}(0) | \psi_0 \rangle \, \delta_{\vec{k},\vec{p}_n/\hbar}$$: veja Eq. (142.3)

$$= \sum_n \int d^3(\vec{r}-\vec{r}') \, e^{-i\vec{k}\cdot(\vec{r}-\vec{r}')} \underbrace{e^{i\vec{p}_n\cdot\vec{r}/\hbar} \langle \psi_0 | \hat{\psi}_{\alpha}(0) | \psi_n \rangle}_{\langle \psi_0 | \hat{\psi}_{\alpha}(\vec{r}) | \psi_n \rangle} \, *$$

: veja pg. 141

$$* \underbrace{e^{-i\vec{p}_n\cdot\vec{r}'/\hbar} \langle \psi_n | \hat{\psi}^{+}_{\alpha}(0) | \psi_0 \rangle}_{\langle \psi_n | \psi^{+}_{\alpha}(\vec{r}') \psi_0 \rangle}$$

$$= \int d^3(\vec{r}-\vec{r}') \, \langle \psi_0 | \psi_{\alpha}(\vec{r}) \, \psi^{+}_{\alpha}(\vec{r}') | \psi_0 \rangle$$

similar p/ 2º termo Eq. (147.1)!

$$\hookrightarrow \int_0^{\infty} d\omega' \left(A(\vec{k},\omega') + B(\vec{k},\omega') \right) =$$

$$= \int d^3(\vec{r}-\vec{r}') \, \langle \psi_0 | \underbrace{\left(\psi_{\alpha}(\vec{r}) \, \psi^{+}_{\alpha}(\vec{r}') + \psi^{+}_{\alpha}(\vec{r}') \, \psi_{\alpha}(\vec{r}) \right)}_{\delta(\vec{r}-\vec{r}')} | \psi_0 \rangle = 1$$

↳ Definição ($\omega \in \mathbb{R}$), veja Eq. (7.25), AGD:

$$\mathrm{Re}\, G = \mathrm{Re}\, G^R = \mathrm{Re}\, G^A$$
$$\mathrm{Im}\, G^R = \mathrm{sgn}(\omega - \mu/\hbar)\, \mathrm{Im}\, G \qquad (148.1)$$
$$\mathrm{Im}\, G^A = -\,\mathrm{sgn}(\omega - \mu/\hbar)\, \mathrm{Im}\, G$$

verifica-se que (veja pg. 148.1):

$$G^R_{\alpha\alpha}(\vec{k},\omega) = \int_0^\infty d\omega' \left(\frac{A(\vec{k},\omega')}{\omega - \omega' - \mu/\hbar + i\eta} + \frac{B(\vec{k},\omega')}{\omega + \omega' - \mu/\hbar + i\eta} \right) \qquad (148.2)$$

e $G^A_{\alpha\alpha}(\vec{k},\omega) = \left(G^R_{\alpha\alpha}(\vec{k},\omega) \right)^*$

na representação de coordenadas, i.e., similar Eq. (127.2), temos que:

$$i G^R_{\alpha\beta}(\vec{r},t;\vec{r}',t') = \Theta(t-t') \langle \Psi_0 | \{ \Psi_\alpha(\vec{r},t) ; \Psi^\dagger_\beta(\vec{r}',t') \} | \Psi_0 \rangle$$
$$(148.3)$$
$$i G^A_{\alpha\beta}(\vec{r},t;\vec{r}',t') = -\Theta(t'-t) \langle \Psi_0 | \{ \Psi_\alpha(\vec{r},t) ; \Psi^\dagger_\beta(\vec{r}',t') \} | \Psi_0 \rangle$$

notar: anticomutador

Exercício: repetir procedimento (140.1) - (146.1) e verificar que Eq. (148.3) → (148.2)!

· Detalhes Eq. (148.2);

Eq. (146.1) p/ $\hbar = 1$ e omitindo índice α:

$$G(\vec{k},\omega) = \int_0^\infty d\omega' \left(\frac{A(\vec{k},\omega')}{\omega - \omega' - \mu + i\eta} + \frac{B(\vec{k},\omega')}{\omega + \omega' - \mu - i\eta} \right)$$

$$= P\int_0^\infty d\omega \left(\frac{A(\vec{k},\omega')}{\omega - \omega' - \mu} + \frac{B(\vec{k},\omega')}{\omega + \omega' - \mu} \right)$$

$$\underbrace{- i\pi A(\vec{k},\omega-\mu)\,\Theta(\omega-\mu)}_{sgn(\omega-\mu)>0} \quad + \underbrace{i\pi B(\vec{k},\mu-\omega)\,\Theta(\mu-\omega)}_{sgn(\omega-\mu)<0}$$

Eq. (148.1)

$\hookrightarrow$ $G^R(\vec{k},\omega) = Re\, G(\vec{k},\omega) - i\pi A(\vec{k},\omega-\mu)\,\Theta(\omega-\mu)$

$$- i\pi B(\vec{k},\mu-\omega)\,\Theta(\mu-\omega)$$

$=$ Eq. (148.2)

· sobre os polos da função de Green interagente;
p/ férmions livres, vimos que, Eq. (134.2):

$$G_{\alpha\alpha}(\vec{k},t) = -i\, e^{-i\epsilon(\vec{k})t/\hbar}\left(\theta(t)\,\theta(k-k_F) - \theta(-t)\,\theta(k_F-k)\right);$$

em particular, p/ $t>0$:

$$G_{\alpha\alpha}(\vec{k},t) = -i\, e^{-i\epsilon(\vec{k})t/\hbar}\,\theta(k-k_F) \qquad (149.1)$$

$\hookrightarrow G_{\alpha\alpha}(\vec{k},\omega) = \dfrac{\theta(k-k_F)}{\omega - \epsilon(\vec{k})/\hbar + i\eta}$: apresenta polo ordem 1 em $\omega = \epsilon(\vec{k})/\hbar - i\eta$

p/ o sistema interagente, é interessante escrever $G(\vec{k},t)$ como (índice α omitido):

$$G(\vec{k},t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, G(\vec{k},\omega) \qquad (149.2)$$

$$= \underbrace{\int_{-\infty}^{\mu/\hbar} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, G(\vec{k},\omega)} + \underbrace{\int_{\mu/\hbar}^{+\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, G(\vec{k},\omega)}$$

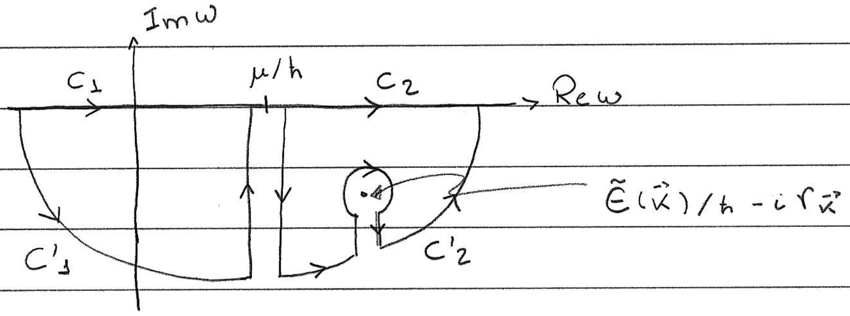
como $\omega < \mu/\hbar$ — como $\mu/\hbar < \omega$

$\hookrightarrow \mathrm{sgn}(\omega - \mu/\hbar) < 0$ — $\hookrightarrow \mathrm{sgn}(\omega-\mu/\hbar) > 0$

Veja Eq. (148.1): $\hookrightarrow G(\vec{k},\omega) = G^A(\vec{k},\omega)$ — $\hookrightarrow G(\vec{k},\omega) = G^R(\vec{k},\omega)$

Lembrar: $G^A(\vec{k},\omega)$: analítica no semi-plano inferior
e $G^R(\vec{k},\omega)$: apresenta polos apenas no semi-plano inferior;

hipótese: $G^R(\vec{k},\omega)$: apresenta apenas 1 polo de ordem 1
em $\omega = \tilde{E}(\vec{k})/\hbar - i\Gamma_{\vec{k}}$; (149.3)



(150.1)

· a integral (149.2) pode ser determinada por resíduos; como $t > 0$ e Eq. (147.1), é interessante deformar as curvas $C_1 \to C'_1$ e $C_2 \to C'_2$, pois as integrais ao longo dos arcos são nulas; temos que:

$$G(\vec{k},t) = \underbrace{\int_{\mu/\hbar - i\infty}^{\mu/\hbar} \frac{d\omega}{2\pi} e^{-i\omega t} \left(G^A(\vec{k},\omega) - G^R(\vec{k},\omega) \right)}_{}$$

↳ 0 p/ $\frac{\hbar}{\tilde{E}(\vec{k}) - \mu} \ll t \ll \frac{\hbar}{\Gamma_{\vec{k}}}$: Veja Eq. (7.80), Fetter

$$+ \underbrace{\oint \frac{d\omega}{2\pi} e^{-i\omega t} G^R(\vec{k},\omega)}_{}$$

$$\frac{1}{2\pi} \cdot 2\pi i (-1) Z_{\vec{k}} e^{-i\tilde{E}(\vec{k})t/\hbar} e^{-\Gamma_{\vec{k}} t}$$

clockwise

resíduo ~ $G^R(\vec{k},\omega)$

↳ $G(\vec{k},t) \approx -i Z_{\vec{k}} e^{-i\tilde{E}(\vec{k})t/\hbar} e^{-\Gamma_{\vec{k}} t}$; $\frac{\hbar}{\tilde{E}(\vec{k})-\mu} \ll t \ll \frac{t}{\Gamma_{\vec{k}}}$ (150.2)

e $\tilde{E}(\vec{k}) - \mu \gg \hbar \Gamma_{\vec{k}}$:

: polo próximo ao eixo Re ω!

· notar: Eq. (150.2) : similar Eq. (149.1)

↳ interpretação: o estado excitado do sistema interagente c/ uma partícula adicional é similar ao correspondente estado do sistema não-interagente, porém:

a energia da excitação $\tilde{E}(\vec{k})$ é renormalizada;

a excitação apresenta uma meia-vida $\hbar/\Gamma_{\vec{k}}$ e

peso (resíduo) $Z_{\vec{k}} \neq 1$
↳ estado excitado do sistema interagente c/ uma partícula adicional: quasipartícula;

· considerações análogas p/ $t<0$: quasiburaco

Obs.: informações experimentais sobre a função de Green de 1 partícula podem ser obtidas via
(veja Cap. 9, Coleman p/ detalhes):

- angle resolved photoemission spectroscopy (ARPES);
- angle integrated " " (AIPES);
- inverse photoemission spectroscopy.