FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

2º Semestre de 2023

14/09/2023

Aula 12

Aula passada

Função de Green de um corpo ordenada temporalmente a T=0:

$$iG_{\alpha\beta}\left(\mathbf{r}t;\mathbf{r}'t'\right) = \frac{\langle\Psi_{0H}|\,T\left[\psi_{H\alpha}\left(\mathbf{r},t\right)\psi^{\dagger}_{H\beta}\left(\mathbf{r}',t'\right)\right]|\Psi_{0H}\rangle}{\langle\Psi_{0H}|\Psi_{0H}\rangle}$$

$$= \theta\left(t-t'\right)\frac{\langle\Psi_{0H}|\,\psi_{H\alpha}\left(\mathbf{r},t\right)\psi^{\dagger}_{H\beta}\left(\mathbf{r}',t'\right)|\Psi_{0H}\rangle}{\langle\Psi_{0H}|\Psi_{0H}\rangle}$$

$$+\zeta\theta\left(t'-t\right)\frac{\langle\Psi_{0H}|\,\psi^{\dagger}_{H\beta}\left(\mathbf{r}',t'\right)\psi_{H\alpha}\left(\mathbf{r},t\right)|\Psi_{0H}\rangle}{\langle\Psi_{0H}|\Psi_{0H}\rangle}$$

$$\boxed{\zeta = \begin{cases} +1, & \text{bósons} \\ -1, & \text{férmions} \end{cases}}$$

Aula passada

Propriedades:

(a) Sistema isolado:

$$G_{\alpha\beta}\left(\mathbf{r}t;\mathbf{r}'t'\right) = G_{\alpha\beta}\left(\mathbf{r},\mathbf{r}',t-t'\right)$$

(b) Invariância translacional:

$$G_{\alpha\beta}\left(\mathbf{r}t;\mathbf{r}'t'\right) = G_{\alpha\beta}\left(\mathbf{r}-\mathbf{r}',t-t'\right) \equiv G_{\alpha\beta}\left(\mathbf{R},T\right)$$

(c) Reversão temporal (ausência de campo magnético ou de magnetização):

$$G_{\alpha\beta}\left(\mathbf{r}t;\mathbf{r}'t'\right) = \delta_{\alpha\beta}G\left(\mathbf{r}-\mathbf{r}',t-t'\right) \equiv \delta_{\alpha\beta}G\left(\mathbf{R},T\right)$$

Valores esperados de operadores de um corpo

i) MATRIZ DENSIDADE DE UM CORPO:

$$\rho_{\alpha\beta}(\vec{r},\vec{r}\,') = \langle \psi^\dagger_\beta(\vec{r}\,')\,\psi_\alpha(\vec{r})\rangle = \frac{\langle \Psi_0|\psi^\dagger_\beta(\vec{r}\,')\,\psi_\alpha(\vec{r})|\Psi_0\rangle}{\langle \Psi_0|\Psi_0\rangle}$$

NA VERSÃO DE SCHRÖDINGER:

$$\lim_{t'\to t^+}[iG_{\alpha\beta}(\vec{r},t;\vec{r}\,',t')] = \mathfrak{z}\,\frac{\langle \Psi_{0H}|\psi^\dagger_{\beta H}(\vec{r}\,',t)\,\psi_{\alpha H}(\vec{r},t)|\Psi_{0H}\rangle}{\langle \Psi_{0H}|\Psi_{0H}\rangle} =$$

$$= \mathfrak{z}\,\frac{\langle \Psi_0|\psi^\dagger_\beta(\vec{r}\,')\,\psi_\alpha(\vec{r})|\Psi_0\rangle}{\langle \Psi_0|\Psi_0\rangle}$$

$$\Rightarrow \rho_{\alpha\beta}(\vec{r},\vec{r}\,') = i\,\mathfrak{z}\lim_{t'\to t^+} G_{\alpha\beta}(\vec{r},t;\vec{r}\,',t')$$

QUALQUER VALOR ESPERADO DE OP. DE UM CORPO PODE SER ESCRITO EM TERMOS DA MAT. DENS. DE UM CORPO. SEJA:

$$\hat{U} = \sum_{\alpha\beta} \int d^3r \, \psi^\dagger_\alpha(\vec{r}) \, U_{\alpha\beta}(\vec{r}) \, \psi_\beta(\vec{r})$$

POR EXEMPLO: ENERGIA POTENCIAL: $U_{\alpha\beta}(\vec{r}) = \delta_{\alpha\beta} V(\vec{r})$

" CINÉTICA: $U_{\alpha\beta}(\vec{r}) = \delta_{\alpha\beta}\left(-\frac{\nabla^2}{2m}\right)$

MAGNET. TOTAL: $U_{\alpha\beta}(\vec{r}) = \frac{\vec{\sigma}_{\alpha\beta}}{2}$

NÚMERO TOTAL: $U_{\alpha\beta}(\vec{r}) = \delta_{\alpha\beta}$

$$\Rightarrow \langle \hat{U} \rangle = \sum_{\alpha\beta} \int d^3r \, \langle \psi^\dagger_\alpha(\vec{r}) \, U_{\alpha\beta}(\vec{r}) \, \psi_\beta(\vec{r}) \rangle$$

$$= \sum_{\alpha\beta} \int d^3r \, \lim_{\vec{r}\,' \to \vec{r}} U_{\alpha\beta}(\vec{r}) \, \langle \psi^\dagger_\alpha(\vec{r}\,') \psi_\beta(\vec{r}) \rangle$$

ASSIM:

$$\langle \hat{U} \rangle = \mp i \sum_{\alpha\beta} \int d^3r \lim_{\vec{r}' \to \vec{r}} \lim_{t' \to t^+} U_{\alpha\beta}(\vec{r})\, G_{\beta\alpha}(\vec{r}, t; \vec{r}', t')$$

Valores esperados no estado fundamental de operadores de um corpo:

$$\widehat{\mathcal{O}} = \sum_{\alpha\beta} \int d^3r \psi_\alpha^\dagger(\mathbf{r})\, U_{\alpha\beta}(\mathbf{r})\, \psi_\beta(\mathbf{r})$$

$$\boxed{\langle \Psi_0 | \, \widehat{\mathcal{O}} \, | \Psi_0 \rangle = \zeta i \sum_{\alpha\beta} \int d^3r \lim_{\eta \to 0^+} \lim_{\mathbf{r} \to \mathbf{r}'} \left[U_{\alpha\beta}(\mathbf{r})\, G_{\beta\alpha}(\mathbf{r}t; \mathbf{r}'t + \eta) \right]}$$

Função de Green não interagente

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

FÉRMIONS EM NÚMERO DE $\underline{N}$: $\quad \dfrac{k_F^3}{3\pi^2} = \dfrac{N}{V}$ (spin 1/2)

$$\psi(\vec{r}) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\, c_{\vec{k}}, \ \ldots \qquad G^{(0)}_{\alpha\beta} = \delta_{\alpha\beta}\, G^{(0)}$$

$$i\,G^{(0)}(\underset{\vec{r},t}{x}, \underset{\vec{r}',t'}{x'}) = \theta(t-t')\langle \Phi_0 | \psi_H(x)\, \psi^\dagger_H(x') | \Phi_0 \rangle$$

$$- \theta(t'-t)\langle \Phi_0 | \psi^\dagger_H(x')\, \psi_H(x) | \Phi_0 \rangle$$

$$\psi_H(\vec{r},t) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\, e^{iH_0 t}\, c_{\vec{k}}\, e^{-iH_0 t} = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\, c_{\vec{k}H}$$

$$c_{\vec{k}H} = e^{it\sum_{\vec{k}'} \epsilon_{\vec{k}'} \hat{n}_{\vec{k}'}}\, c_{\vec{k}}\, e^{-it\sum_{\vec{p}} \epsilon_{\vec{p}} \hat{n}_{\vec{p}}} = e^{it\epsilon_{\vec{k}} \hat{n}_{\vec{k}}}\, c_{\vec{k}}\, e^{-it\epsilon_{\vec{k}} \hat{n}_{\vec{k}}}$$

USANDO BAKER-HAUSDORFF: $e^{A} B e^{-A} = B + [A,B] + \frac{1}{2!}[A,[A,B]] + \dots$

$$[c_{\vec{k}}, \hat{n}_{\vec{k}}] = [c_{\vec{k}}, c^{\dagger}_{\vec{k}} c_{\vec{k}}] = \{c_{\vec{k}}, c^{\dagger}_{\vec{k}}\} c_{\vec{k}} - c^{\dagger}_{\vec{k}} \{c_{\vec{k}}, c_{\vec{k}}\}$$

$$[A, BC] = [A,B]_{\xi} C + \xi B [A, C]_{\xi}$$

ALTERNATIVAMENTE, ATUANDO NOS ESTADOS $|n_k=0\rangle$ E $|n_k=1\rangle$:

$$e^{it\epsilon_{\vec{k}}\hat{n}_{\vec{k}}} c_{\vec{k}} e^{-it\epsilon_{\vec{k}}\hat{n}_{\vec{k}}} = e^{-it\epsilon_{\vec{k}}} c_{\vec{k}}$$

$$\psi_H(\vec{r},t) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}} e^{-i\epsilon_{\vec{k}} t}}{\sqrt{V}} c_{\vec{k}}$$

ASSIM:

$$iG^{(0)}(x,x') = \frac{\theta(t-t')}{V} \sum_{\vec{k},\vec{p}} e^{i\vec{k}\cdot\vec{r}} e^{-i\vec{p}\cdot\vec{r}'} e^{-i\epsilon_{\vec{k}} t} e^{+i\epsilon_{\vec{p}} t'} \langle \Phi_0 | c_{\vec{k}} c^{\dagger}_{\vec{p}} | \Phi_0 \rangle$$

$$- \frac{\theta(t'-t)}{V} \sum_{\vec{k},\vec{p}} e^{i\vec{k}\cdot\vec{r}} e^{-i\vec{p}\cdot\vec{r}'} e^{-i\epsilon_{\vec{k}} t} e^{+i\epsilon_{\vec{p}} t'} \langle \Phi_0 | c^{\dagger}_{\vec{p}} c_{\vec{k}} | \Phi_0 \rangle$$

$$\langle \Phi_0 | c_{\vec{k}} c^{\dagger}_{\vec{p}} | \Phi_0 \rangle = \delta_{\vec{p},\vec{k}} \theta(k-k_F) ; \quad \langle \Phi_0 | c^{\dagger}_{\vec{p}} c_{\vec{k}} | \Phi_0 \rangle = \delta_{\vec{p},\vec{k}} \theta(k_F-k)$$

$$iG^{(0)}(x,x') = \frac{1}{V}\sum_{\vec{k}} e^{i\vec{k}\cdot\underbrace{(\vec{r}-\vec{r}')}_{\vec{R}}}\, e^{-i\epsilon_{\vec{k}}\underbrace{(t-t')}_{T}}\left[\theta(\underbrace{t-t'}_{T})\theta(k-k_F)-\right.$$

$$\left.-\theta(\underbrace{t'-t}_{-T})\theta(k_F-k)\right]$$

$$G^{(0)}(\vec{k}',\omega) = \int \underbrace{d^3(\vec{r}-\vec{r}')}_{d^3R}\, \underbrace{d(t-t')}_{dT}\, e^{-i\vec{k}'\cdot\overbrace{(\vec{r}-\vec{r}')}^{\vec{R}}}\, e^{i\omega\overbrace{(t-t')}^{T}}\, G^{(0)}(\underbrace{\vec{r}-\vec{r}'}_{\vec{R}};\underbrace{t-t'}_{T})$$

$$\int \frac{d^3R}{V} e^{-i\vec{k}'\cdot\vec{R}} e^{i\vec{k}\cdot\vec{R}} = \delta^{(3)}(\vec{k}-\vec{k}')$$

$$iG^{(0)}(\vec{k};T) = e^{-i\epsilon_{\vec{k}}T}\left[\theta(T)\theta(k-k_F)-\theta(-T)\theta(k_F-k)\right]$$

$$G^{(0)}(\vec{k},\omega) = \int dT\, e^{i\omega T} e^{-i\epsilon_{\vec{k}}T}\left[-i\theta(T)\theta(k-k_F)+i\theta(-T)\theta(k_F-k)\right]$$

$$= \theta(k-k_F)\int_0^\infty dT\,(-i)\,e^{i(\omega-\epsilon_{\vec{k}})T} + \theta(k_F-k)\int_{-\infty}^0 dT\,(i)\,e^{i(\omega-\epsilon_{\vec{k}})T}$$

$$= \theta(k-k_F)\int_0^\infty dT\,(-i)\,e^{i(\omega+i\eta-\epsilon_{\vec{k}})T} + \theta(k_F-k)\int_{-\infty}^0 dT\,(i)\,e^{i(\omega-i\eta-\epsilon_{\vec{k}})T}$$

ONDE $\eta \to 0^+$

FAZENDO AS INTEGRAIS:

$$G^{(0)}(\vec{k},\omega) = \frac{\theta(k-k_F)}{\omega-\epsilon_{\vec{k}}+i\eta} + \frac{\theta(k_F-k)}{\omega-\epsilon_{\vec{k}}-i\eta}$$

$$\boxed{G^{(0)}_{\alpha\beta}(\vec{k},\omega) = \frac{\delta_{\alpha\beta}}{\omega-\epsilon_{\vec{k}}+i\eta\,\mathrm{sgn}(k-k_F)}}$$

NOTEM A ESTRUTURA DE PÓLOS SIMPLES DE $G^{(0)}_{\alpha\beta}(\vec{k},\omega)$ NO PLANO COMPLEXO DE ω NAS ENERGIAS DO SISTEMA Ñ INTERAGENTE.

PÓLOS: $\omega = \epsilon_{\vec{k}} - \underbrace{i\eta\,\mathrm{sgn}(k-k_F)}$

LOGO ABAIXO (ACIMA) DO EIXO DE $\underline{\omega}$ REAL PARA PARTÍCULA (BURACO).

Função de Green não interagente (férmions):

$$\boxed{iG^{(0)}_{\alpha\beta}\left(\mathbf{r}t;\mathbf{r}'t'\right)=\frac{\delta_{\alpha\beta}}{V}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}e^{-i\epsilon(\mathbf{k})(t-t')}\left[\theta\left(t-t'\right)\theta\left(k-k_F\right)-\theta\left(t'-t\right)\theta\left(k_F-k\right)\right]}$$

$$\begin{aligned}G_{\alpha\beta}\left(\mathbf{k},\omega\right) &= \int d^3RdTe^{-i\mathbf{k}\cdot\mathbf{R}}e^{i\omega T}G_{\alpha\beta}\left(\mathbf{R},T\right)\\ G_{\alpha\beta}\left(\mathbf{R},T\right) &= \int \frac{d^3kd\omega}{\left(2\pi\right)^4}e^{i\mathbf{k}\cdot\mathbf{R}}e^{-i\omega T}G_{\alpha\beta}\left(\mathbf{k},\omega\right)\end{aligned}$$

$$G^{(0)}_{\alpha\beta}\left(\mathbf{k},\omega\right)=\delta_{\alpha\beta}G^{(0)}\left(\mathbf{k},\omega\right)$$

$$\boxed{G^{(0)}\left(\mathbf{k},\omega\right) = \frac{1}{\omega-\epsilon\left(\mathbf{k}\right)+i\eta\,\mathrm{sgn}\left(k-k_F\right)}}$$

Valor esperado de um operador de dois corpos a partir da função de Green

USANDO DERIVADAS TEMPORAIS DE $\psi_H(\vec{r}, t)$

$$i\partial_t \psi_H(\vec{r},t) = [\psi_H(\vec{r},t), H]$$

PARA:

$$H = \sum_\alpha \int d^3r\, \psi^\dagger_\alpha(\vec{r}) \left(-\frac{\nabla^2}{2m}\right)\psi_\alpha(\vec{r}) + \frac{1}{2}\sum_{\alpha\beta}\int d^3r\, d^3r'\, \psi^\dagger_\alpha(\vec{r})\psi^\dagger_\beta(\vec{r}')V(\vec{r}-\vec{r}')\psi_\beta(\vec{r}')\psi_\alpha(\vec{r}) = \hat{H}_0 + \hat{V}$$

$$i\partial_t \psi_{\alpha H}(x) = -\frac{\nabla^2}{2m}\psi_{\alpha H}(x) + \sum_\beta \int d^3r'\, V(\vec{r}-\vec{r}')\psi^\dagger_{\beta H}(\vec{r}',t)\psi_{\beta H}(\vec{r}',t)\psi_{\alpha H}(x)$$

$$\Rightarrow \langle \hat{V} \rangle = \frac{1}{2}\int d^3r \lim_{\substack{\vec{r}'\to\vec{r} \\ t'\to t^+}} \sum_\alpha \left(i\partial_t + \frac{\nabla^2}{2m}\right)(i\mathfrak{I})G_{\alpha\alpha}(\vec{r}t;\vec{r}'t')$$

$$\langle \hat{H} \rangle = \langle \hat{H}_0 \rangle + \langle \hat{V} \rangle =$$

$$= \frac{1}{2} \int d^3 r \lim_{\substack{\vec{r}\,' \to \vec{r} \\ t' \to t^+}} \sum_{\alpha} \left(i\partial_t - \frac{\nabla^2}{2m} \right) (i \mathfrak{Z}) G_{\alpha\alpha}(\vec{r}\,t; \vec{r}\,'; t')$$

Valor esperado de um operador de dois corpos a partir da função de Green

Sistema homogêneo com interação de pares:

$$H = \sum_{\alpha} \int d^3r \psi_{\alpha}^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \psi_{\alpha}(\mathbf{r}) + \underbrace{\frac{1}{2} \sum_{\alpha\beta} \int d^3r d^3r' \psi_{\alpha}^{\dagger}(\mathbf{r}) \psi_{\beta}^{\dagger}(\mathbf{r}') U(\mathbf{r}-\mathbf{r}') \psi_{\beta}(\mathbf{r}') \psi_{\alpha}(\mathbf{r})}_{U}$$

$$\boxed{\langle U \rangle = \frac{i\zeta}{2} \sum_{\alpha} \int d^3r \lim_{t' \to t^+} \lim_{\mathbf{r} \to \mathbf{r}'} \left[\left(i\partial_t + \frac{\hbar^2\nabla^2}{2m}\right) G_{\alpha\alpha}(\mathbf{r}t; \mathbf{r}'t')\right]}$$

$$\boxed{\langle H \rangle = \frac{i\zeta}{2} \sum_{\alpha} \int d^3r \lim_{t' \to t^+} \lim_{\mathbf{r} \to \mathbf{r}'} \left[\left(i\partial_t - \frac{\hbar^2\nabla^2}{2m}\right) G_{\alpha\alpha}(\mathbf{r}t; \mathbf{r}'t')\right]}$$

$t' \to t + \eta \qquad \eta \to 0^+$

RECORRENDO À TRANSFORMADAS DE FOURIER NO ESPAÇO E NO TEMPO:

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

PODEMOS ESCREVER AS FÓRMULAS ANTERIORES COMO: $(\eta \to 0^+)$

$$\langle \hat{H}_0 \rangle = \zeta i V \sum_{\alpha} \int \frac{d^3k\,d\omega}{(2\pi)^4}\, e^{i\omega\eta}\, G_{\alpha\alpha}(\vec{k},\omega)\left(\frac{k^2}{2m}\right)$$

$$\langle \hat{W} \rangle = \zeta i V \sum_{\alpha} \int \frac{d^3k\,d\omega}{(2\pi)^4}\, e^{i\omega\eta}\, G_{\alpha\alpha}(\vec{k},\omega)$$

$$\langle \hat{H} \rangle = \frac{\zeta i V}{2} \sum_{\alpha} \int \frac{d^3k\,d\omega}{(2\pi)^4} \left[\omega + \frac{k^3}{2m}\right] e^{i\omega\eta}\, G_{\alpha\alpha}(\vec{k},\omega)$$

$$\langle \vec{S} \rangle = \frac{\zeta i V}{2} \sum_{\alpha\beta} \int \frac{d^3k\,d\omega}{(2\pi)^4}\, e^{i\omega\eta}\, \vec{\sigma}_{\beta\alpha}\, G_{\alpha\beta}(\vec{k},\omega)$$

$$\mathrm{Tr}[\vec{\sigma}\, G]$$