FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

2º Semestre de 2023

19/10/2023

Aula 19

Algumas aproximações clássicas

A aproximação Hartree-Fock

$$\hat{H}_0 = \int d^3x\, \hat{\psi}^\dagger_\alpha(\mathbf{x}) \left[-\frac{\hbar^2 \nabla^2}{2m} + U(\mathbf{x}) \right] \hat{\psi}_\alpha(\mathbf{x})$$

$$\hat{H}_1 = \tfrac{1}{2} \int d^3x\, d^3x'\, \hat{\psi}^\dagger_\alpha(\mathbf{x})\, \hat{\psi}^\dagger_\beta(\mathbf{x}')\, V(\mathbf{x}-\mathbf{x}')\, \hat{\psi}_\beta(\mathbf{x}')\, \hat{\psi}_\alpha(\mathbf{x})$$

TÉCNICA COMUM DE CÁLCULO DE EST. ELETRÔNICA.

$$\Psi(x_1, x_2 \cdots x_N) = \begin{vmatrix} \varphi_1(x_1) & \varphi_1(x_2) & \varphi_1(x_3) \cdots & \varphi_1(x_N) \\ \varphi_2(x_1) & \varphi_2(x_2) & \cdots & \vdots \\ \vdots & & & \vdots \\ \varphi_N(x_1) & \varphi_N(x_2) & \cdots & \varphi_N(x_N) \end{vmatrix}$$

FUNÇÃO DE ONDA ANTI-SIMETRIZADA PARA <u>N</u> FÉRMIONS OCUPANDO <u>N</u> ORBITAIS DE PARTÍCULA ÚNICA.

COMO OTIMIZAR PARA A MELHOR ESCOLHA DOS ORBITAIS.

$\langle H \rangle = \langle \Phi | H | \Phi \rangle$ SUJEITO A $\langle \Phi | \Phi \rangle = 1$

$$\frac{\delta \langle H \rangle}{\delta \varphi_i(x_i)} = 0 \Rightarrow \text{EQS. HARTREE-FOCK.}$$

Equações Hartree-Fock

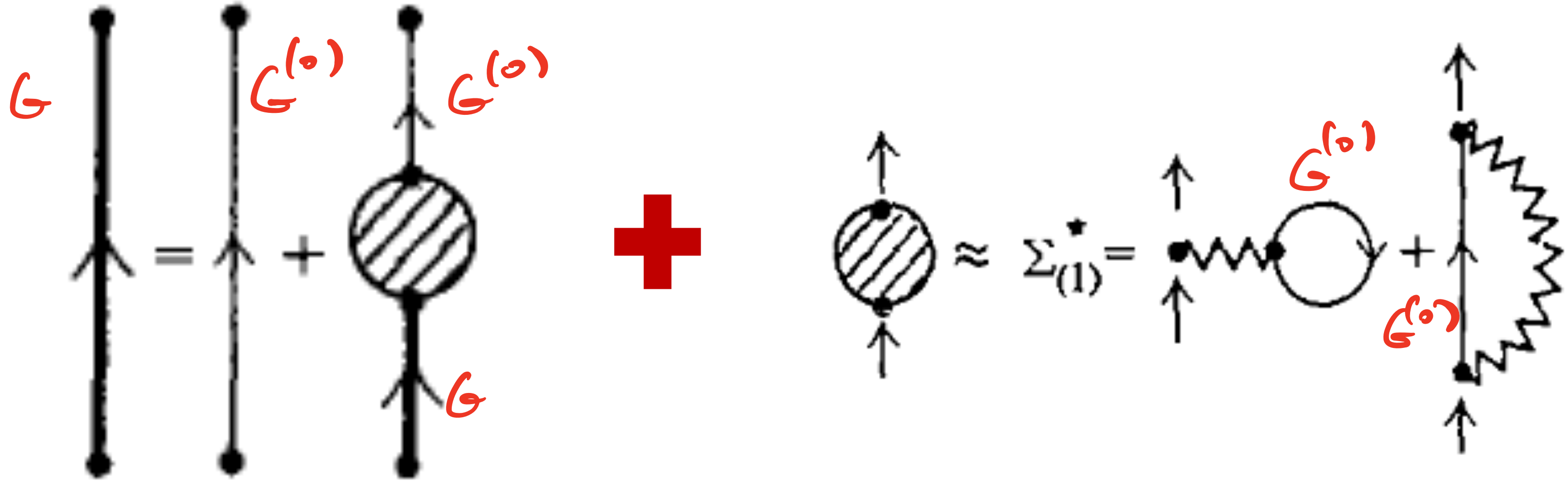
Equações auto-consistentes:

$$\left[-\frac{\hbar^2\nabla_1^2}{2m}+U\left(\mathbf{x}_1\right)\right]\varphi_i\left(\mathbf{x}_1\right)+$$

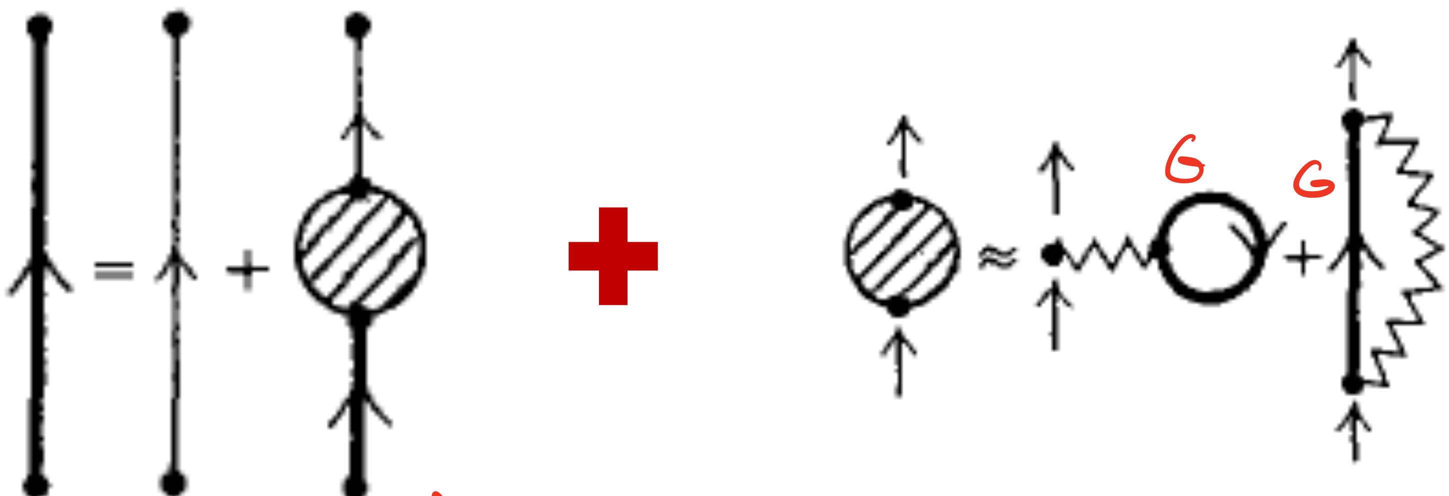
$$\sum_j\left[\int d^3x_2 V\left(\mathbf{x}_1-\mathbf{x}_2\right)\left|\varphi_j\left(\mathbf{x}_2\right)\right|^2\theta\left(E_F-\epsilon_j\right)\right]\varphi_i\left(\mathbf{x}_1\right)-$$

$$\sum_j\left[\int d^3x_2 V\left(\mathbf{x}_1-\mathbf{x}_2\right)\varphi_j^*\left(\mathbf{x}_2\right)\varphi_i\left(\mathbf{x}_2\right)\theta\left(E_F-\epsilon_j\right)\right]\varphi_j\left(\mathbf{x}_1\right) \;=\; \epsilon_i\varphi_i\left(\mathbf{x}_1\right)$$

Auto-energia em primeira ordem:

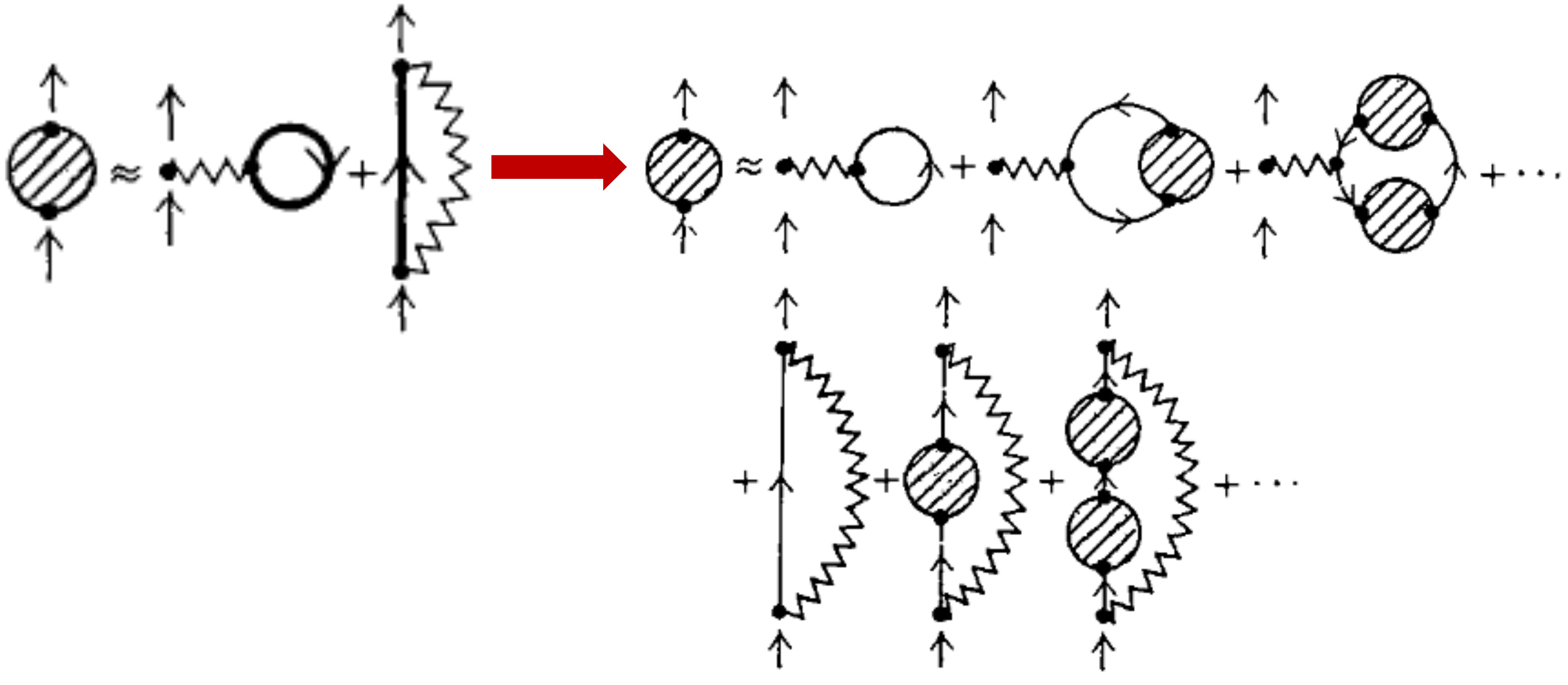


Aproximação Hartree-Fock: auto-consistência



ESSE SISTEMA É EQUIVALENTE ÀS EQS. H-F (F+W, P. 121-127)

Aproximação Hartree-Fock: infinitas ordens incluídas na auto-energia



Férmions num potencial externo

$$\hat{H}_0 = \int d^3x\, \hat{\psi}^\dagger_\alpha(\mathbf{x}) \left[-\frac{\hbar^2 \nabla^2}{2m} + U(\mathbf{x}) \right] \hat{\psi}_\alpha(\mathbf{x})$$

$$\hat{H}_1 = \frac{1}{2} \int d^3x\, d^3x'\, \hat{\psi}^\dagger_\alpha(\mathbf{x})\, \hat{\psi}^\dagger_\beta(\mathbf{x}')\, V(\mathbf{x} - \mathbf{x}')\, \hat{\psi}_\beta(\mathbf{x}')\, \hat{\psi}_\alpha(\mathbf{x})$$

Ver desenvolvimento no Fetter & Walecka, pags. 121-127

$$\left[-\frac{\hbar^2}{2m}\frac{\nabla_1^2}{} + U(\mathbf{x}_1)\right]\varphi_j(\mathbf{x}_1) + \int d^3x_2\, \hbar\Sigma^\star(\mathbf{x}_1,\mathbf{x}_2)\,\varphi_j(\mathbf{x}_2) = \epsilon_j\,\varphi_j(\mathbf{x}_1)$$

$$\hbar\Sigma^\star(\mathbf{x}_1,\mathbf{x}_1') = \delta(\mathbf{x}_1 - \mathbf{x}_1')\int d^3x_2\, V(\mathbf{x}_1 - \mathbf{x}_2)\, n(\mathbf{x}_2) - V(\mathbf{x}_1 - \mathbf{x}_1')\sum_j \varphi_j(\mathbf{x}_1)\,\varphi_j(\mathbf{x}_1')^*\,\theta(\epsilon_F - \epsilon_j)$$

$$\left[-\frac{\hbar^2\nabla_1^2}{2m} + U\left(\mathbf{x}_1\right)\right]\varphi_i\left(\mathbf{x}_1\right) + \sum_j \left[\int d^3x_2 V\left(\mathbf{x}_1 - \mathbf{x}_2\right)\left|\varphi_j\left(\mathbf{x}_2\right)\right|^2\theta\left(E_F - \epsilon_j\right)\right]\varphi_i\left(\mathbf{x}_1\right) - \sum_j \left[\int d^3x_2 V\left(\mathbf{x}_1 - \mathbf{x}_2\right)\varphi_j^*\left(\mathbf{x}_2\right)\varphi_i\left(\mathbf{x}_2\right)\theta\left(E_F - \epsilon_j\right)\right]\varphi_j\left(\mathbf{x}_1\right) = \epsilon_i\varphi_i\left(\mathbf{x}_1\right)$$

Sistema homogêneo

SE $U(\bar{x}) = 0$. A BASE DE ONDAS PLANAS SEMPRE RESOLVE O PROBLEMA HOMOGÊNEO.

LEVANDO: $\varphi_i(\bar{x}) = \dfrac{e^{i\vec{k}_i \cdot \vec{r}}}{\sqrt{V}}$ NA AUTO-ENERGIA $\Sigma(x_1, x_2)$

RECUPERAMOS: $\Sigma^{(1)}(\vec{k})$ JÁ VISTA.

O gás de elétrons de alta densidade: a "random phase approximation" (RPA)

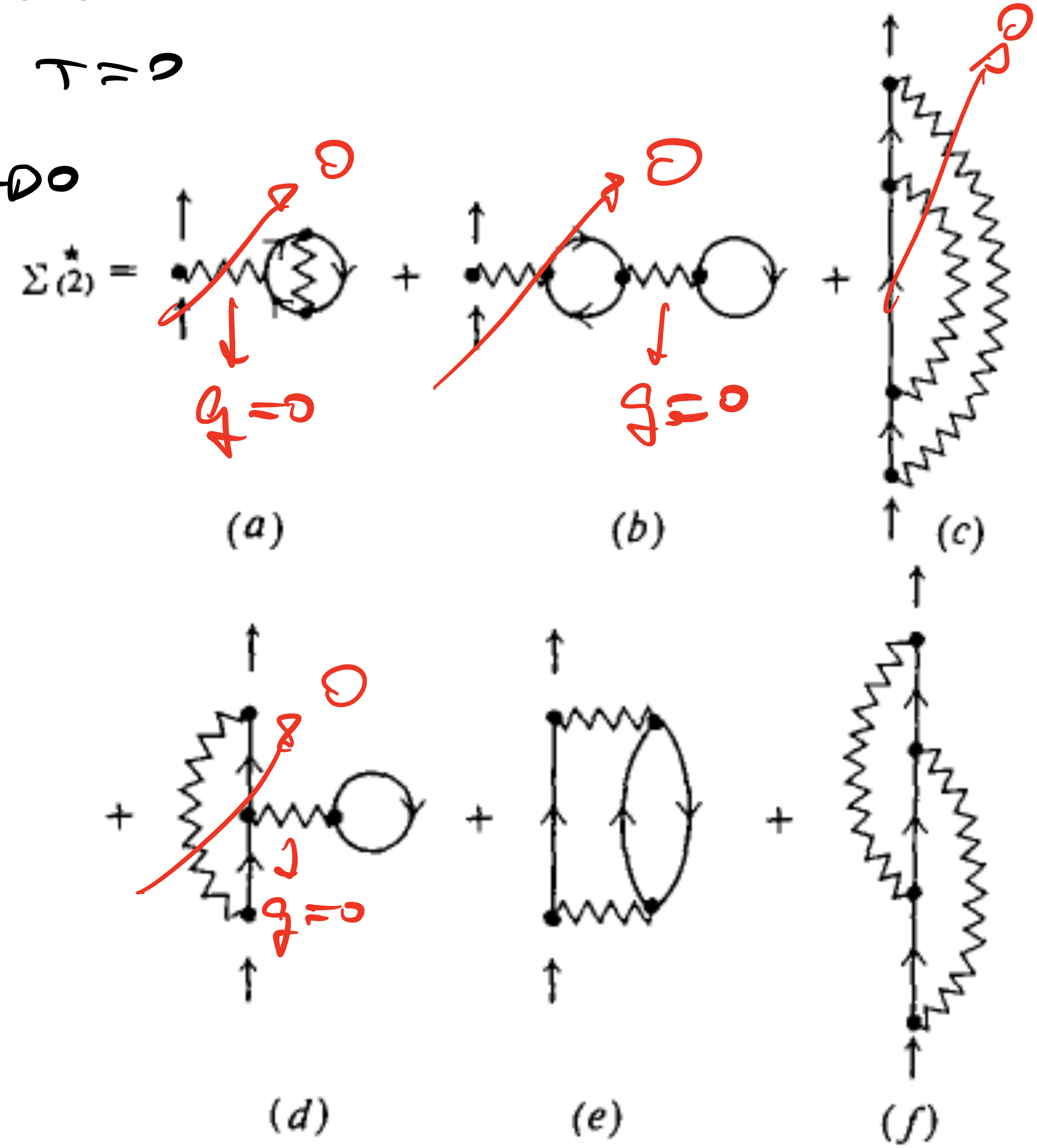
O GÁS DE ELÉTRONS EM $T=0$ É UNICAMENTE DETERMINADO POR SUA DENSIDADE:

$$\frac{N}{V} = \frac{k_F^3}{3\pi^2}$$

$$\frac{4}{3}\pi (r_s a_0)^3 = \frac{V}{N} = \frac{3\pi^2}{k_F^3}$$

ALTA DENSIDADE: $r_s \ll 1$

$$\Rightarrow k_F \sim r_s^{-1}$$

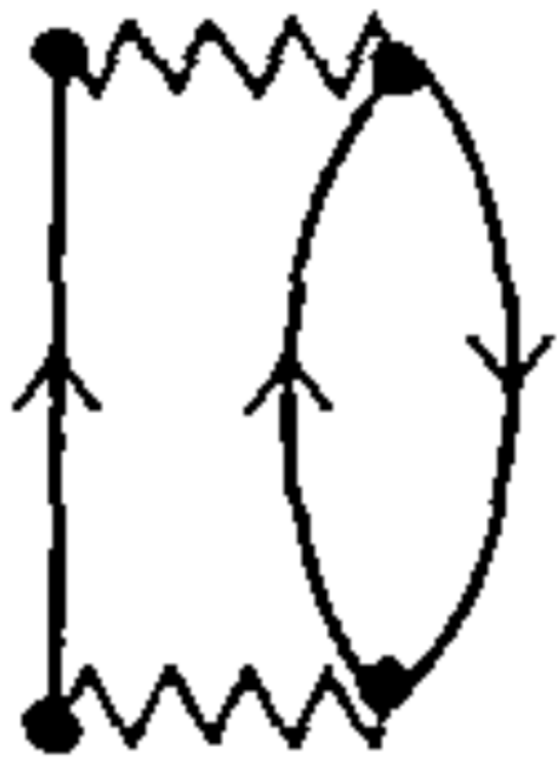


$$\Sigma^{(2a)}(\vec{k},\omega) = 2\int \frac{d^3q\, d^3p\, d\nu\, d\epsilon}{(2\pi)^8} \frac{(4\pi e^2)^2}{q^4} G^{(0)}(\vec{k}-\vec{q},\omega-\epsilon)$$

$$G^{(0)}(\vec{p},\nu)\, G^{(0)}(\vec{p}+\vec{q}, \nu+\epsilon)$$

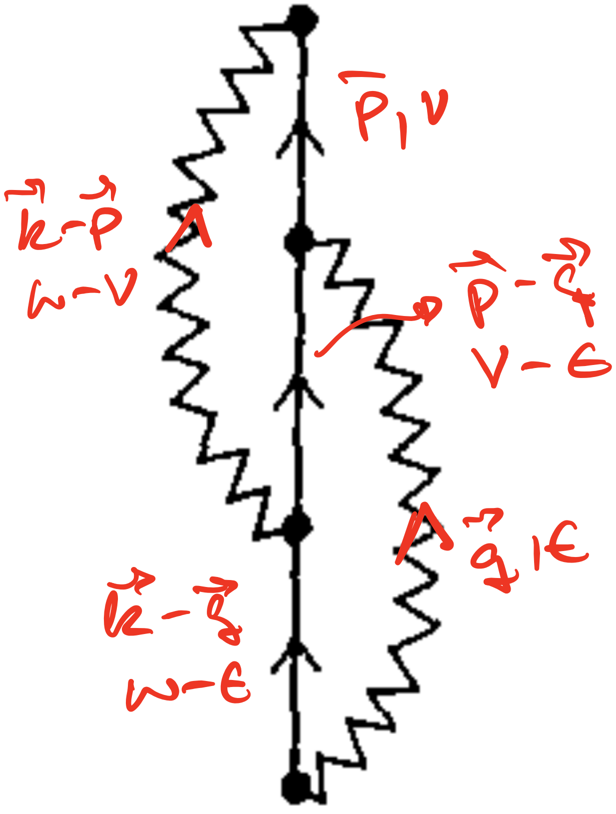
A INTEGRAÇÃO SOBRE $\underline{\nu}$, $\underline{\epsilon}$ É

IMEDIATA



$$\Sigma^{(2a)}(\omega,\mathbf{k}) = 2\int \frac{d^3q d^3p}{(2\pi)^6}\left(\frac{4\pi e^2}{q^2}\right)^2 \left[\frac{\theta(|\mathbf{k}-\mathbf{q}|-k_F)\,\theta(|\mathbf{p}+\mathbf{q}|-k_F)\,\theta(k_F-p)}{\omega-\epsilon(\mathbf{k}-\mathbf{q})-\epsilon(\mathbf{p}+\mathbf{q})+\epsilon(\mathbf{p})+i\eta}\right.$$

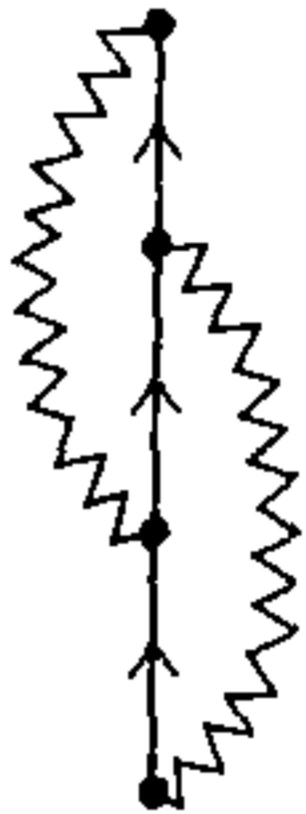
$$\left. + \frac{\theta(k_F-|\mathbf{k}-\mathbf{q}|)\,\theta(k_F-|\mathbf{p}+\mathbf{q}|)\,\theta(p-k_F)}{\omega-\epsilon(\mathbf{k}-\mathbf{q})-\epsilon(\mathbf{p}+\mathbf{q})+\epsilon(\mathbf{p})-i\eta}\right]$$



$$\Sigma^{(2b)}(\vec{k},\omega) = -\int \frac{d^3q\, d^3p\, d\nu\, d\epsilon}{(2\pi)^8} \frac{(4\pi e^2)^2}{q^2(\vec{k}-\vec{p})^2}$$

$$G^{(0)}(\vec{k}-\vec{q}, \omega-\epsilon)\, G^{(0)}(\vec{p}, \nu)\, G^{(0)}(\vec{p}-\vec{q}, \nu-\epsilon)$$

INTEGRA-SE SOBRE $\underline{\nu}, \underline{\epsilon}$



$$\Sigma^{(2b)}(\omega,\mathbf{k}) = \int \frac{d^3q d^3p}{(2\pi)^6}\frac{\left(4\pi e^2\right)^2}{q^2\left|\mathbf{k}-\mathbf{p}\right|^2}\left[\frac{\theta\left(k_F-|\mathbf{k}-\mathbf{q}|\right)\theta\left(|\mathbf{p}-\mathbf{q}|-k_F\right)\theta\left(k_F-p\right)}{\omega-\epsilon\left(\mathbf{k}-\mathbf{q}\right)+\epsilon\left(\mathbf{p}-\mathbf{q}\right)-\epsilon\left(\mathbf{p}\right)+i\eta}\right.$$

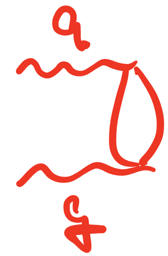
$$\left.+\frac{\theta\left(|\mathbf{k}-\mathbf{q}|-k_F\right)\theta\left(k_F-|\mathbf{p}-\mathbf{q}|\right)\theta\left(p-k_F\right)}{\omega-\epsilon\left(\mathbf{k}-\mathbf{q}\right)+\epsilon\left(\mathbf{p}-\mathbf{q}\right)-\epsilon\left(\mathbf{p}\right)-i\eta}\right]$$

Graus de divergência

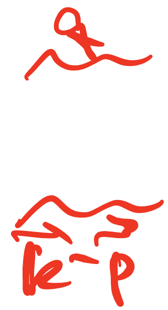
NOS 2 DIAGRAMAS $\Sigma^{(2a)}$, $\Sigma^{(2b)}$ O TERMO ENTRE COLCHETES É FINITO QUANDO $q \to 0$ (VAMOS MOSTRAR ISSO MAIS TARDE)

ASSIM:

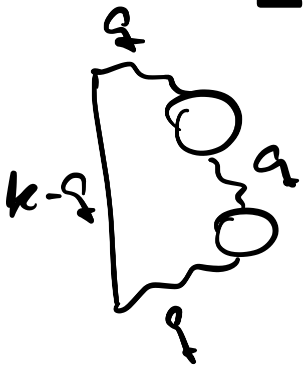
$$\Sigma^{(2a)} \sim \int \frac{d^3q}{q^4} \sim \int \frac{q^2\,dq}{q^4} \sim \int \frac{dq}{q^2} \xrightarrow[q\to 0]{} \infty \Rightarrow$$



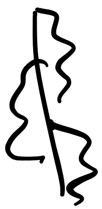
$$\Sigma^{(2b)} \sim \int \frac{d^3q}{q^2} \sim \int dq \underset{q\to 0}{<} \infty \qquad \Rightarrow$$



Em 3ª ordem de T. de Pert.

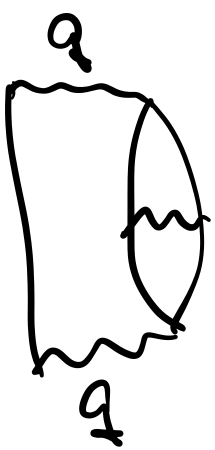


$$\sim \int \frac{d^3q}{q^6} \sim \int \frac{dq}{q^4} \to \infty$$



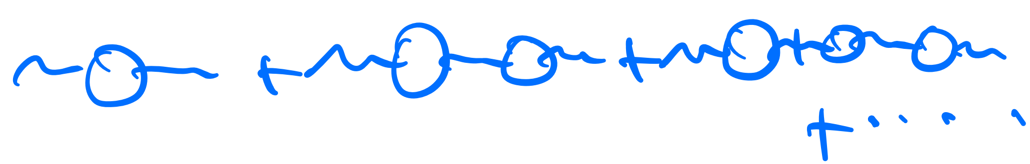
$$\sim \int \frac{d^3q}{q^2} < \infty$$

ETC.



$$\sim \int \frac{d^3q}{q^4} \sim \int \frac{dq}{q^2} \to \infty$$

CLARAMENTE, EM ORDENS SUPERIORES, AS DIVERGÊNCIAS MAIS SEVERAS VIRÃO DE:



Análise dimensional

$G^{(0)} \sim \frac{1}{\omega - \varepsilon_k} \sim \frac{1}{k_F^2}$ $\quad U(q) \sim \frac{1}{k_F^2}$ $\quad \int d^4q \sim \int d^3q\, d\nu \sim k_F^5$

2ª ORDEM: $\left[G^{(0)}\right]^3 U^2 \int d^4q\, d^4p \sim k_F^{-6}\, k_F^{-4}\, k_F^{10} \sim (k_F)^0 \sim (r_s)^0$

3ª ORDEM: $(2^{a}\text{ ORDEM})\, U \left[G^{(0)}\right]^2 \int d^4q \sim k_F^{-2}\, k_F^{-4}\, k_F^{5} \sim k_F^{-1} \sim r_s$

UMA ORDEM A MAIS INTRODUZ MAIS UMA POTÊNCIA DE r_s

nª ORDEM: $(r_s)^{n-2}$

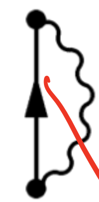
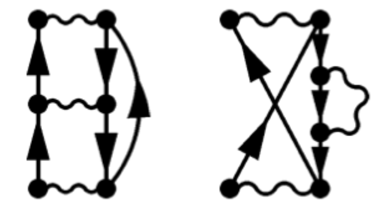
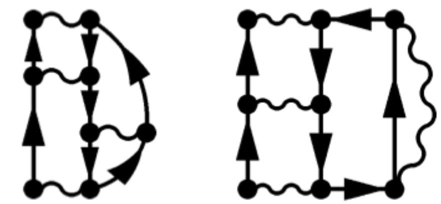
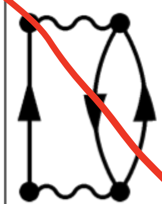
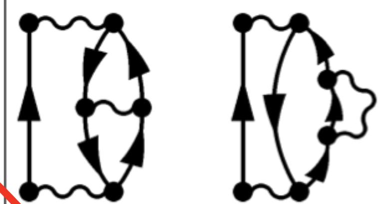
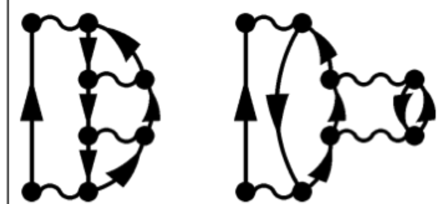
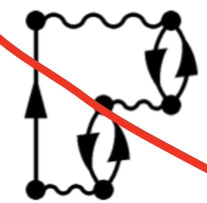
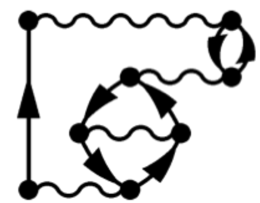
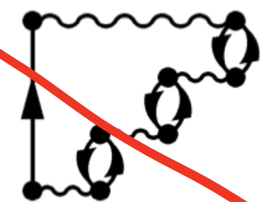
– VAMOS QUERER INCLUIR OS DIAGRAMAS COM MAIOR GRAU DE DIVERGÊNCIA E MENORES POTÊNCIAS DE r_s (NO LIMITE DE ALTA DENSIDADE)

Ordem em teoria de perturbação

NÃO DIVERGENTES

$\int \frac{dq}{q^2}$

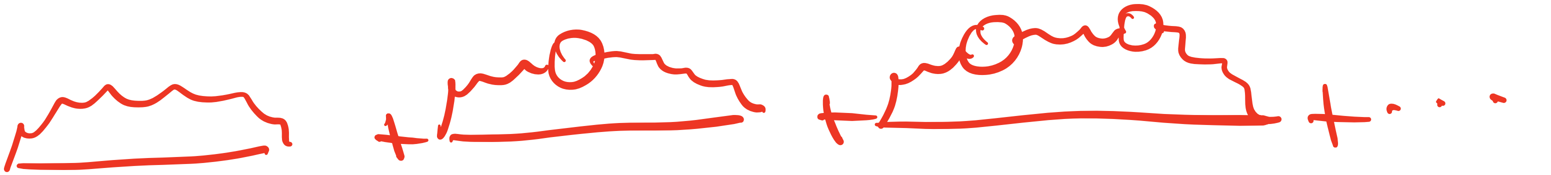
Grau de diverg. (δ)

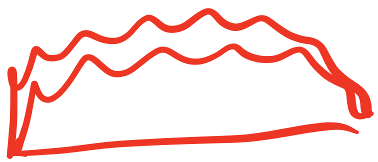
$\Sigma_\sigma(\tilde{k})$	$n = 1$	$n = 2$	$n = 3$	$n = 4$
$\delta = 1$				
$\delta = 2$	–			
$\delta = 3$	–	–		
$\delta = 4$	–	–	–	

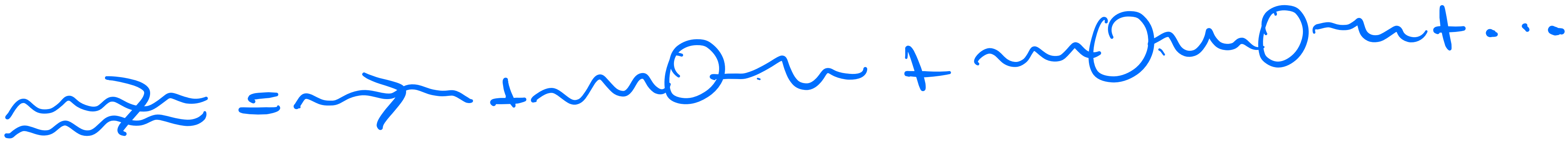
LINHA A SER MANTIDA

A auto-energia em alta densidade

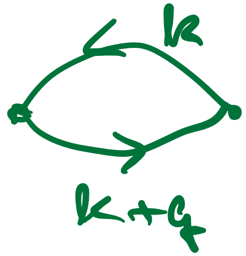
$\Sigma^{AD} =$  $+ \; \Sigma^{RPA}$

$\Sigma^{RPA} =$ 

$=$ 

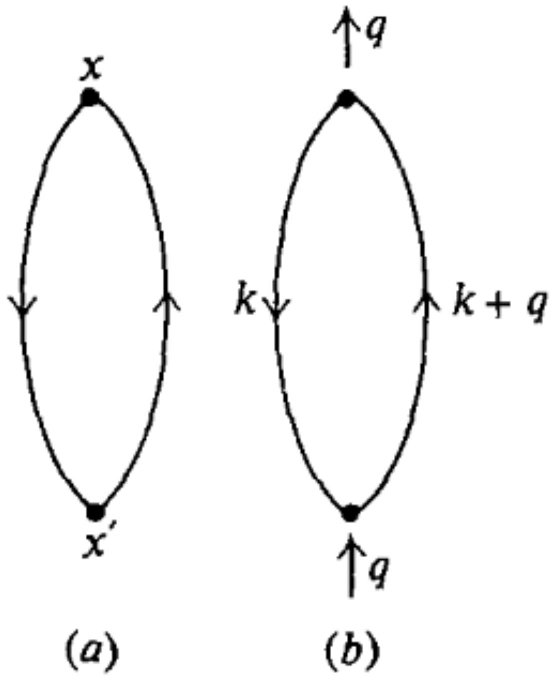


$$U^R(q) = \frac{U(q)}{1 - U(q)\,\Pi^{(0)}(q)} = \frac{4\pi e^2/q^2}{1 - \frac{4\pi e^2}{q^2}\Pi^{(0)}(q)} = \frac{4\pi e^2}{q^2 - 4\pi e^2\,\Pi^{(0)}(q)}$$

$\Pi^{(0)}(q) =$ 

$$= -2i \int \frac{d^3k\, d\omega}{(2\pi)^4}\, G^{(0)}(\vec{k},\omega)\, G^{(0)}(\vec{k}+\vec{q},\omega+\nu)$$

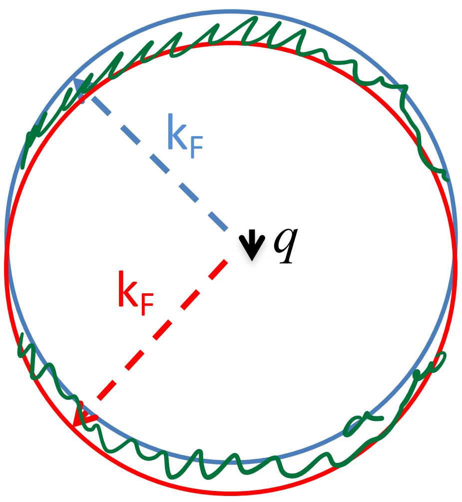
A função de Lindhard



$$
\begin{aligned}
\Pi^0(\mathbf{q},\nu) &= -2i\int \frac{d^3k\,d\omega}{(2\pi)^4} G^{(0)}(\mathbf{k},\omega)\,G^{(0)}(\mathbf{k}+\mathbf{q},\omega+\nu) \\
&= 2\int \frac{d^3k}{(2\pi)^3}\left[\frac{\theta(k_F-k)\,\theta(|\mathbf{k}+\mathbf{q}|-k_F)}{\nu+\epsilon(\mathbf{k})-\epsilon(\mathbf{k}+\mathbf{q})+i\eta}-\frac{\theta(k-k_F)\,\theta(k_F-|\mathbf{k}+\mathbf{q}|)}{\nu+\epsilon(\mathbf{k})-\epsilon(\mathbf{k}+\mathbf{q})-i\eta}\right]
\end{aligned}
$$

A função de Lindhard no limite estático

$$\Pi^0(\mathbf{q},0) = 2\int \frac{d^3k}{(2\pi)^3}\left[\frac{\theta(k_F-k)\,\theta(|\mathbf{k}+\mathbf{q}|-k_F)}{\epsilon(\mathbf{k})-\epsilon(\mathbf{k}+\mathbf{q})+i\eta} - \frac{\theta(k-k_F)\,\theta(k_F-|\mathbf{k}+\mathbf{q}|)}{\epsilon(\mathbf{k})-\epsilon(\mathbf{k}+\mathbf{q})-i\eta}\right]$$



$q << k_F$:

$$\epsilon(k)-\epsilon(\vec{k}+\vec{q}) = \frac{k^2}{2m} - \frac{|\vec{k}+\vec{q}|^2}{2m} = -\frac{\vec{k}\cdot\vec{q}}{m}$$

$$\theta(k-k_F)\,\theta(k_F-|\vec{k}+\vec{q}|) \simeq \delta(k-k_F)\,(-q\cos\theta) \qquad \left(\frac{\pi}{2}<\theta<\pi\right)$$

$$\theta(k_F-k)\,\theta(|\vec{k}+\vec{q}|-k_F) \simeq \delta(k-k_F)\,q\cos\theta \qquad \left(0<\theta<\frac{\pi}{2}\right)$$

$$\Pi^{(0)}(\vec{q},0) = 2\int\underbrace{\frac{d^3k}{(2\pi)^3}}_{2\pi k^2 dk\, d(\cos\theta)} \frac{\delta(k-k_F)\,\cancel{q\cos\theta}}{-k_F\cancel{q\cos\theta}/m} = -\frac{2mk_F}{4\pi^2}\times 2 = -\frac{mk_F}{\pi^2}$$

$$= -g(E_F)$$

$$U^R(\vec{q}) = \frac{4\pi e^2}{q^2 - 4\pi e^2\left(-\frac{mk_F}{\pi^2}\right)} = \frac{4\pi e^2}{q^2 + q_{TF}^2}$$

$$q_{TF}^2 = 4\pi e^2 g_F = \frac{4 e^2 m k_F}{\pi} = \left(\frac{4}{\pi}\right)\left(\frac{4}{9\pi}\right)^{1/3} r_s k_F^2 \simeq 0.66\, r_s k_F^2$$

$q_{TF} = \sqrt{0.66\, r_s}\, k_F$ = VETOR DE ONDA DE THOMAS-FERMI

$$U^R(r) = \frac{e^2}{r} e^{-q_{TF} r}$$

BLINDAGEM DE THOMAS-FERMI

Gás de elétrons

LEVANDO $U^R(q)$ EM Σ^{RPA}

$\tilde{\epsilon}(k) = \frac{k_F}{m^*}(k - k_F)$

$$\frac{m^*}{m} = 1 + 0.083 r_s (\ln r_s + 0.203)$$

$$2\gamma_k = \frac{1}{\tau_k} = 0.252\sqrt{r_s}\frac{(k-k_F)^2}{2m}$$

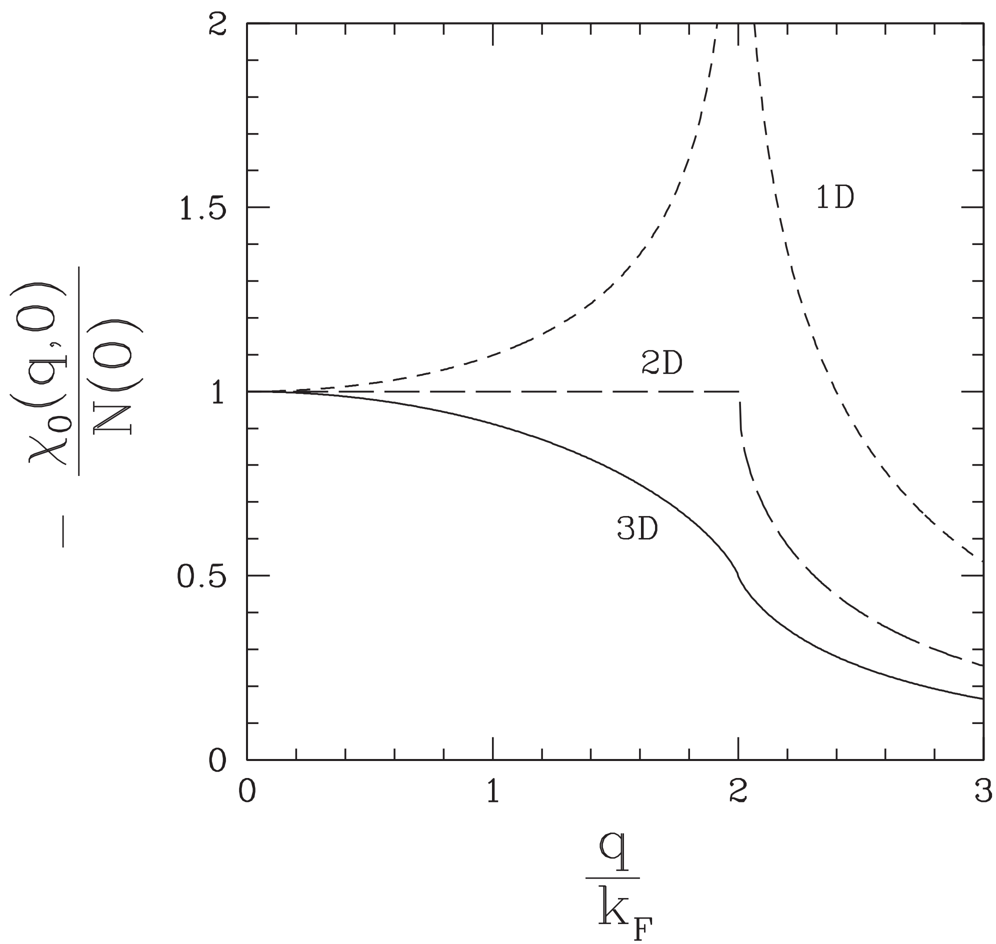
$$\epsilon(r_s) \simeq \begin{cases} \left(\frac{2.210}{r_s^2} - \frac{0.916}{r_s} + 0.062\ln r_s - 0.093 + \mathcal{O}(r_s \ln r_s)\right) \text{ Ry}, & (3D), \\ \left(\frac{1}{r_s^2} - \frac{1.20}{r_s} - (0.38 \pm 0.04) - 0.1726\, r_s \ln r_s + \mathcal{O}(r_s)\right) \text{ Ry}, & (2D). \end{cases}$$

$\epsilon(r_s) = \frac{E(r_s)}{N}$

Função de Lindhard no limite estático

Table 4.2. *Explicit expressions for $\chi_{0\sigma}(q,0)$ – the static limit of the one-spin Lindhard function. Here $\bar{q}_\sigma = \frac{q}{k_{F\sigma}}$. The corresponding Fourier transforms are given in Table 4.3.*

d	$\chi_{0\sigma}(q,0)$
3	$-N_\sigma(0)\left[\frac{1}{2} + \frac{\bar{q}_\sigma^2 - 4}{8\bar{q}_\sigma}\ln\left\lvert\frac{\bar{q}_\sigma - 2}{\bar{q}_\sigma + 2}\right\rvert\right]$
2	$-N_\sigma(0)\left[1 - \Theta(\bar{q}_\sigma - 2)\frac{\sqrt{\bar{q}_\sigma^2 - 4}}{\bar{q}_\sigma}\right]$
1	$-N_\sigma(0)\left[\frac{1}{\bar{q}_\sigma}\ln\left\lvert\frac{\bar{q}_\sigma + 2}{\bar{q}_\sigma - 2}\right\rvert\right]$



Quantum theory of the electron liquid,

Gabriele Giuliani, Giovanni Vignale, Cambridge University Press, 2005.