

$$H = H_{el} + H_b + H_{el-b}$$

REPASO

$$H_{el} = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{1}{2} e^2 \sum_{i \neq j}^N \frac{e^{-\mu |\mathbf{r}_i - \mathbf{r}_j|}}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$H_b = \frac{1}{2} e^2 \iint d^3x d^3x' \frac{n(\mathbf{x}) n(\mathbf{x}') e^{-\mu |\mathbf{x} - \mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|}$$

$$H_{el-b} = -e^2 \sum_{i=1}^N \int d^3x \frac{n(\mathbf{x}) e^{-\mu |\mathbf{x} - \mathbf{r}_i|}}{|\mathbf{x} - \mathbf{r}_i|}$$

# Gas de electrones: Jellium model

El Hamiltoniano quedó reducido a:  $H = -\frac{1}{2}e^2 N^2 V^{-1} 4\pi\mu^{-2} + H_{el}$

REPASO

$$H_{el} = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{1}{2} e^2 \sum_{i \neq j}^N \frac{e^{-\mu|\mathbf{r}_i - \mathbf{r}_j|}}{|\mathbf{r}_i - \mathbf{r}_j|}$$

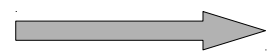
Ahora pasamos a **segunda cuantización**.

$$\hat{F} = \sum_{k,l} \langle u_k | \hat{f} | u_l \rangle a_k^\dagger a_l$$

Término de **Energía cinética**:

$$\begin{aligned} \langle \mathbf{k}_1 \lambda_1 | T | \mathbf{k}_2 \lambda_2 \rangle &= (2mV)^{-1} \int d^3x e^{-i\mathbf{k}_1 \cdot \mathbf{x}} \eta_{\lambda_1}^\dagger (-\hbar^2 \nabla^2) e^{i\mathbf{k}_2 \cdot \mathbf{x}} \eta_{\lambda_2} \\ &= \frac{\hbar^2 k_2^2}{2mV} \delta_{\lambda_1 \lambda_2} \int d^3x e^{i(\mathbf{k}_2 - \mathbf{k}_1) \cdot \mathbf{x}} \\ &= \frac{\hbar^2 k_2^2}{2m} \delta_{\lambda_1 \lambda_2} \delta_{\mathbf{k}_1 \mathbf{k}_2} \end{aligned}$$

$$\int d^3x e^{i(\mathbf{k}_2 - \mathbf{k}_1) \cdot \mathbf{x}} = V \delta_{\mathbf{k}_1 \mathbf{k}_2}$$



$$\hat{T} = \sum_{\mathbf{k}\lambda} \frac{\hbar^2 k^2}{2m} a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda}$$

# Gas de electrones: Jellium model

REPASO

$$\begin{aligned} \langle \mathbf{k}_1 \lambda_1 \mathbf{k}_2 \lambda_2 | V | \mathbf{k}_3 \lambda_3 \mathbf{k}_4 \lambda_4 \rangle &= \frac{e^2}{V^2} \iint d^3x_1 d^3x_2 e^{-i\mathbf{k}_1 \cdot \mathbf{x}_1} \eta_{\lambda_1}(1)^\dagger \\ &\quad \times e^{-i\mathbf{k}_2 \cdot \mathbf{x}_2} \eta_{\lambda_2}(2)^\dagger \frac{e^{-\mu|\mathbf{x}_1 - \mathbf{x}_2|}}{|\mathbf{x}_1 - \mathbf{x}_2|} \\ &\quad \times e^{i\mathbf{k}_3 \cdot \mathbf{x}_1} \eta_{\lambda_3}(1) e^{i\mathbf{k}_4 \cdot \mathbf{x}_2} \eta_{\lambda_4}(2) \end{aligned}$$

Sustituyendo:  $\mathbf{x} = \mathbf{x}_2$  and  $\mathbf{y} = \mathbf{x}_1 - \mathbf{x}_2 \longrightarrow \mathbf{x}_1 = \mathbf{y} + \mathbf{x}$

$$\begin{aligned} \langle \mathbf{k}_1 \lambda_1 \mathbf{k}_2 \lambda_2 | V | \mathbf{k}_3 \lambda_3 \mathbf{k}_4 \lambda_4 \rangle &= \frac{e^2}{V^2} \int d^3x e^{-i(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{x}} \\ &\quad \times \int d^3y e^{i(\mathbf{k}_3 - \mathbf{k}_1) \cdot \mathbf{y}} \frac{e^{-\mu y}}{y} \delta_{\lambda_1 \lambda_3} \delta_{\lambda_2 \lambda_4} \\ &= \frac{e^2}{V} \delta_{\lambda_1 \lambda_3} \delta_{\lambda_2 \lambda_4} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4} \frac{4\pi}{(\mathbf{k}_1 - \mathbf{k}_3)^2 + \mu^2} \end{aligned}$$

Example: the Hamiltonian of translationally invariant systems in second quantization

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Universität Würzburg

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Harvard University

O Heinonen  
University of Central Florida

$$v(\mathbf{r}, \mathbf{r}') = v(\mathbf{r} - \mathbf{r}')$$

$$v(\mathbf{r} - \mathbf{r}') = \frac{1}{\Omega} \sum_{\mathbf{q}} v_{\mathbf{q}} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} \quad v_{\mathbf{q}} = \int_{\Omega} d^3\tau v(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}}$$

$$\hat{V} = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N v(\mathbf{r}_i - \mathbf{r}_j) = \frac{1}{2\Omega} \sum_{\mathbf{q}} v_{\mathbf{q}} \sum_{\substack{i,j=1 \\ i \neq j}}^N e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)}$$

$$\phi_{\mathbf{k}\sigma}(\mathbf{x}) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k} \cdot \mathbf{r}} \chi_{\sigma}(s)$$

$$\hat{V} = \frac{1}{2\Omega} \sum_{\mathbf{q}} v_{\mathbf{q}} \sum_{\mathbf{k}_1\sigma_1} \sum_{\mathbf{k}_2\sigma_2} \sum_{\mathbf{k}_3\sigma_3} \sum_{\mathbf{k}_4\sigma_4} \langle \mathbf{k}_1\sigma_1, \mathbf{k}_2\sigma_2 | e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} | \mathbf{k}_3\sigma_3, \mathbf{k}_4\sigma_4 \rangle \times \hat{c}_{\mathbf{k}_1\sigma_1}^{\dagger} \hat{c}_{\mathbf{k}_2\sigma_2}^{\dagger} \hat{c}_{\mathbf{k}_4\sigma_4} \hat{c}_{\mathbf{k}_3\sigma_3}$$

# Gas de electrones: Jellium model

REPASO

$$\hat{H} = -\frac{1}{2} \frac{e^2 N^2 4\pi}{V \mu^2} + \sum_{\mathbf{k}\lambda} \frac{\hbar^2 k^2}{2m} a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda} + \frac{e^2}{2V}$$

$$\times \sum_{\mathbf{k}_1 \lambda_1} \sum_{\mathbf{k}_2 \lambda_2} \sum_{\mathbf{k}_3 \lambda_3} \sum_{\mathbf{k}_4 \lambda_4} \delta_{\lambda_1 \lambda_3} \delta_{\lambda_2 \lambda_4} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4}$$

$$\times \frac{4\pi}{(\mathbf{k}_1 - \mathbf{k}_3)^2 + \mu^2} a_{\mathbf{k}_1 \lambda_1}^\dagger a_{\mathbf{k}_2 \lambda_2}^\dagger a_{\mathbf{k}_4 \lambda_4} a_{\mathbf{k}_3 \lambda_3}$$

<https://blog.cupcakephysics.com/electromagnetism/math%20methods/2014/10/04/the-fourier-transform-of-the-coulomb-potential.html>

$$\begin{matrix} \mathbf{k}_1 = \mathbf{k} + \mathbf{q} & \mathbf{k}_3 = \mathbf{k} \\ \mathbf{k}_2 = \mathbf{p} - \mathbf{q} & \mathbf{k}_4 = \mathbf{p} \end{matrix} \longrightarrow \frac{e^2}{2V} \sum_{\mathbf{k}\mathbf{p}\mathbf{q}} \sum_{\lambda_1 \lambda_2} \frac{4\pi}{q^2 + \mu^2} a_{\mathbf{k}+\mathbf{q}, \lambda_1}^\dagger a_{\mathbf{p}-\mathbf{q}, \lambda_2}^\dagger a_{\mathbf{p}\lambda_2} a_{\mathbf{k}\lambda_1}$$

Separamos el término  $\mathbf{q} = 0$

$$\frac{e^2}{2V} \sum'_{\mathbf{k}\mathbf{p}\mathbf{q}} \sum_{\lambda_1 \lambda_2} \frac{4\pi}{q^2 + \mu^2} a_{\mathbf{k}+\mathbf{q}, \lambda_1}^\dagger a_{\mathbf{p}-\mathbf{q}, \lambda_2}^\dagger a_{\mathbf{p}\lambda_2} a_{\mathbf{k}\lambda_1}$$

$$+ \frac{e^2}{2V} \sum_{\mathbf{k}\mathbf{p}} \sum_{\lambda_1 \lambda_2} \frac{4\pi}{\mu^2} a_{\mathbf{k}\lambda_1}^\dagger a_{\mathbf{p}\lambda_2}^\dagger a_{\mathbf{p}\lambda_2} a_{\mathbf{k}\lambda_1}$$

# Gas de electrones: Jellium model

$$\begin{aligned}
 a_{\mathbf{k}\lambda_1}^\dagger a_{\mathbf{p}\lambda_2}^\dagger a_{\mathbf{p}\lambda_2} a_{\mathbf{k}\lambda_1} &= -a_{\mathbf{k}\lambda_1}^\dagger a_{\mathbf{p}\lambda_2}^\dagger a_{\mathbf{k}\lambda_1} a_{\mathbf{p}\lambda_2} = \\
 &= -a_{\mathbf{k}\lambda_1}^\dagger (-a_{\mathbf{k}\lambda_1} a_{\mathbf{p}\lambda_2}^\dagger + \delta_{\mathbf{k}\lambda_1, \mathbf{p}\lambda_2}) a_{\mathbf{p}\lambda_2} = \\
 &= a_{\mathbf{k}\lambda_1}^\dagger a_{\mathbf{k}\lambda_1} a_{\mathbf{p}\lambda_2}^\dagger a_{\mathbf{p}\lambda_2} - \delta_{\mathbf{k}\lambda_1, \mathbf{p}\lambda_2} a_{\mathbf{k}\lambda_1}^\dagger a_{\mathbf{p}\lambda_2} = \\
 &= n_{\mathbf{k}\lambda_1} n_{\mathbf{p}\lambda_2} - \delta_{\mathbf{k}\lambda_1, \mathbf{p}\lambda_2} n_{\mathbf{k}\lambda_1}
 \end{aligned}$$

El término de q=0 se puede escribir como:

$$\frac{e^2}{2V} \frac{4\pi}{\mu^2} \sum_{\mathbf{k}\lambda_1} \sum_{\mathbf{p}\lambda_2} a_{\mathbf{k}\lambda_1}^\dagger a_{\mathbf{k}\lambda_1} (a_{\mathbf{p}\lambda_2}^\dagger a_{\mathbf{p}\lambda_2} - \delta_{\mathbf{k}\mathbf{p}} \delta_{\lambda_1 \lambda_2}) = \frac{e^2}{2V} \frac{4\pi}{\mu^2} (\hat{N}^2 - \hat{N})$$

Número fijo de partículas:  $\hat{N} \longrightarrow N$

$$\longrightarrow \frac{e^2 N^2 4\pi}{2V \mu^2} - \frac{e^2 N 4\pi}{2V \mu^2}$$

Se cancela con el otro término de H

$$\longrightarrow -\frac{1}{2} 4\pi e^2 (V \mu^2)^{-1} \text{ por partícula}$$

Se va a cero al hacer:  $L \rightarrow \infty$

Y después:  $\mu \rightarrow 0$

# Gas de electrones: Jellium model

Y así obtenemos:

$$\hat{H} = \sum_{\mathbf{k}\lambda} \frac{\hbar^2 k^2}{2m} a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda} + \frac{e^2}{2V} \sum'_{\mathbf{k}\mathbf{p}\mathbf{q}} \sum_{\lambda_1\lambda_2} \frac{4\pi}{q^2} a_{\mathbf{k}+\mathbf{q},\lambda_1}^\dagger a_{\mathbf{p}-\mathbf{q},\lambda_2}^\dagger a_{\mathbf{p}\lambda_2} a_{\mathbf{k}\lambda_1}$$

Adimensionalización. Introducimos  $r_0$  distancia entre partículas:  $V \equiv \frac{4}{3}\pi r_0^3 N$

Radio de Bohr:  $a_0 = \frac{\hbar^2}{me^2} \longrightarrow r_s \equiv \frac{r_0}{a_0}$

$$\bar{V} = r_0^{-3} V \quad \bar{\mathbf{k}} = r_0 \mathbf{k} \quad \bar{\mathbf{p}} = r_0 \mathbf{p} \quad \bar{\mathbf{q}} = r_0 \mathbf{q}$$

$$\hat{H} = \frac{e^2}{a_0 r_s^2} \left( \sum_{\bar{\mathbf{k}}\lambda} \frac{1}{2} \bar{k}^2 a_{\bar{\mathbf{k}}\lambda}^\dagger a_{\bar{\mathbf{k}}\lambda} + \frac{r_s}{2\bar{V}} \sum'_{\bar{\mathbf{k}}\bar{\mathbf{p}}\bar{\mathbf{q}}} \sum_{\lambda_1\lambda_2} \frac{4\pi}{\bar{q}^2} a_{\bar{\mathbf{k}}+\bar{\mathbf{q}},\lambda_1}^\dagger a_{\bar{\mathbf{p}}-\bar{\mathbf{q}},\lambda_2}^\dagger a_{\bar{\mathbf{p}}\lambda_2} a_{\bar{\mathbf{k}}\lambda_1} \right)$$

## Gas de electrones: Jellium model

$$\hat{H} = \frac{e^2}{a_0 r_s^2} \left( \sum_{\mathbf{k}\lambda} \frac{1}{2} k^2 a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda} + \frac{r_s}{2V} \sum_{\mathbf{k}\mathbf{p}\mathbf{q}}' \sum_{\lambda_1 \lambda_2} \frac{4\pi}{q^2} a_{\mathbf{k}+\mathbf{q}, \lambda_1}^\dagger a_{\mathbf{p}-\mathbf{q}, \lambda_2}^\dagger a_{\mathbf{p}\lambda_2} a_{\mathbf{k}\lambda_1} \right)$$

$$r_s \equiv \frac{r_0}{a_0}$$

Esta expresión muestra un resultado anti-intuitivo: a alta densidad, o sea cuando  $r_s \rightarrow 0$  la energía potencial se vuelve una perturbación de la energía cinética.

Entonces, a densidad alta se puede intentar un desarrollo perturbativo de, por ejemplo, la energía del estado fundamental (ground state).

Se obtiene:

$$E = \frac{Ne^2}{a_0 r_s^2} (a + br_s + cr_s^2 \ln r_s + dr_s^2 + \dots)$$

Ahora calculamos a y b.



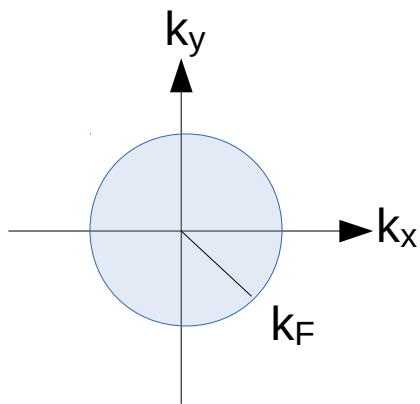
# Gas de electrones: Jellium model

Volvamos al Hamiltoniano con unidades físicas:

$$\hat{H}_0 = \sum_{\mathbf{k}\lambda} \frac{\hbar^2 k^2}{2m} a_{\mathbf{k}\lambda}^\dagger a_{\mathbf{k}\lambda}$$

Electrones no interactuantes:  
exclusión de Pauli, esfera de Fermi

$$\hat{H}_1 = \frac{e^2}{2V} \sum_{\mathbf{k}\mathbf{p}\mathbf{q}} \sum_{\lambda_1\lambda_2} \frac{4\pi}{q^2} a_{\mathbf{k}+\mathbf{q},\lambda_1}^\dagger a_{\mathbf{p}-\mathbf{q},\lambda_2}^\dagger a_{\mathbf{p}\lambda_2} a_{\mathbf{k}\lambda_1}$$



Esfera de Fermi:  $|F\rangle$

Si expandimos la energía:  $E^{(0)} + E^{(1)} + \dots$

$|F\rangle$

Estado fundamental  
no interactuante

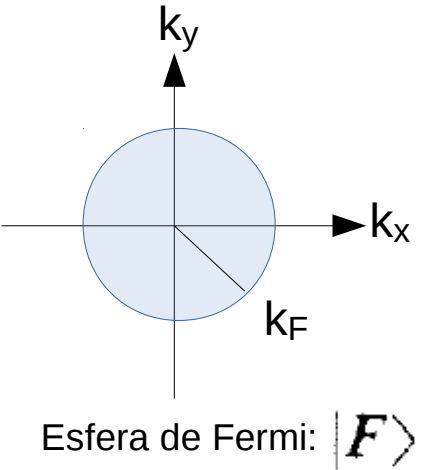
Order cero,  
no interactuante

Corrección a primer order,  
debida a la interacción e-e

$$k_i = \frac{2\pi n_i}{L} \quad i = x, y, z \quad n_i = 0, \pm 1, \pm 2, \dots$$

# Gas de electrones: Jellium model

Estado fundamental  
no interactuante



Calculamos el k de Fermi,  $k_F$  :

$$\begin{aligned}
 N &= \langle F | \hat{N} | F \rangle = \sum_{\mathbf{k}\lambda} \langle F | \hat{n}_{\mathbf{k}\lambda} | F \rangle = \sum_{\mathbf{k}\lambda} \theta(k_F - k) \\
 &= V(2\pi)^{-3} \sum_{\lambda} \int d^3k \theta(k_F - k) = (3\pi^2)^{-1} V k_F^3 = N
 \end{aligned}$$

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

Se usó la densidad de estados en el espacio k que surge de las condiciones periódicas de contorno:

$$k_i = \frac{2\pi n_i}{L} \quad i = x, y, z \quad n_i = 0, \pm 1, \pm 2, \dots$$

$$\begin{aligned}
 \sum_{\mathbf{k}\lambda} f_{\lambda}(\mathbf{k}) &= \sum_{n_x n_y n_z} \sum_{\lambda} f_{\lambda} \left( \frac{2\pi \mathbf{n}}{L} \right) \xrightarrow{L \rightarrow \infty} \iiint dn_x dn_y dn_z \sum_{\lambda} f_{\lambda} \left( \frac{2\pi \mathbf{n}}{L} \right) \\
 &= V(2\pi)^{-3} \sum_{\lambda} \int d^3k f_{\lambda}(\mathbf{k})
 \end{aligned}$$

# Gas de electrones: Jellium model

Estado fundamental  
no interactuante

$|F\rangle$

Dijimos :

$$\begin{aligned} N &= \langle F | \hat{N} | F \rangle = \sum_{\mathbf{k}\lambda} \langle F | \hat{n}_{\mathbf{k}\lambda} | F \rangle = \sum_{\mathbf{k}\lambda} \theta(k_F - k) \\ &= V(2\pi)^{-3} \sum_{\lambda} \int d^3k \theta(k_F - k) = (3\pi^2)^{-1} V k_F^3 = N \end{aligned}$$

Despejemos: El  $k_F$  está fijado por la densidad de electrones:

$$k_F = \left( \frac{3\pi^2 N}{V} \right)^{\frac{1}{3}} = \left( \frac{9\pi}{4} \right)^{\frac{1}{3}} r_0^{-1} \approx 1.92 r_0^{-1}$$

Recordemos el  $r_0$ :  $V \equiv \frac{4}{3}\pi r_0^3 N$

# Gas de electrones: Jellium model

Energía del estado fundamental no interactuante:

$$\begin{aligned} E^{(0)} &= \langle F | \hat{H}_0 | F \rangle = \frac{\hbar^2}{2m} \sum_{\mathbf{k}\lambda} k^2 \langle F | \hat{n}_{\mathbf{k}\lambda} | F \rangle \\ &= \frac{\hbar^2}{2m} \sum_{\mathbf{k}\lambda} k^2 \theta(k_F - k) \\ &= \frac{\hbar^2}{2m} \sum_{\lambda} V (2\pi)^{-3} \int d^3k k^2 \theta(k_F - k) \\ &= \frac{3 \hbar^2 k_F^2}{5 \cdot 2m} N = \frac{e^2}{2a_0} \frac{N}{r_s^2} \frac{3}{5} \left( \frac{9\pi}{4} \right)^{\frac{2}{3}} = \frac{e^2}{2a_0} N \frac{2.21}{r_s^2} \end{aligned}$$

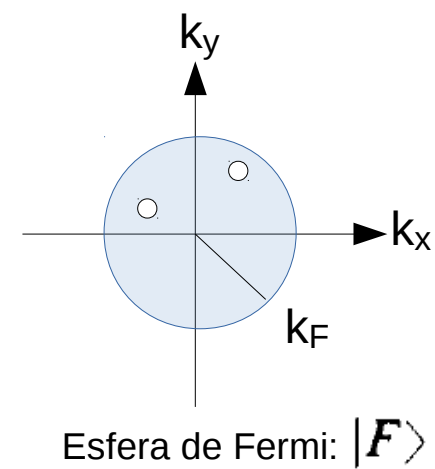
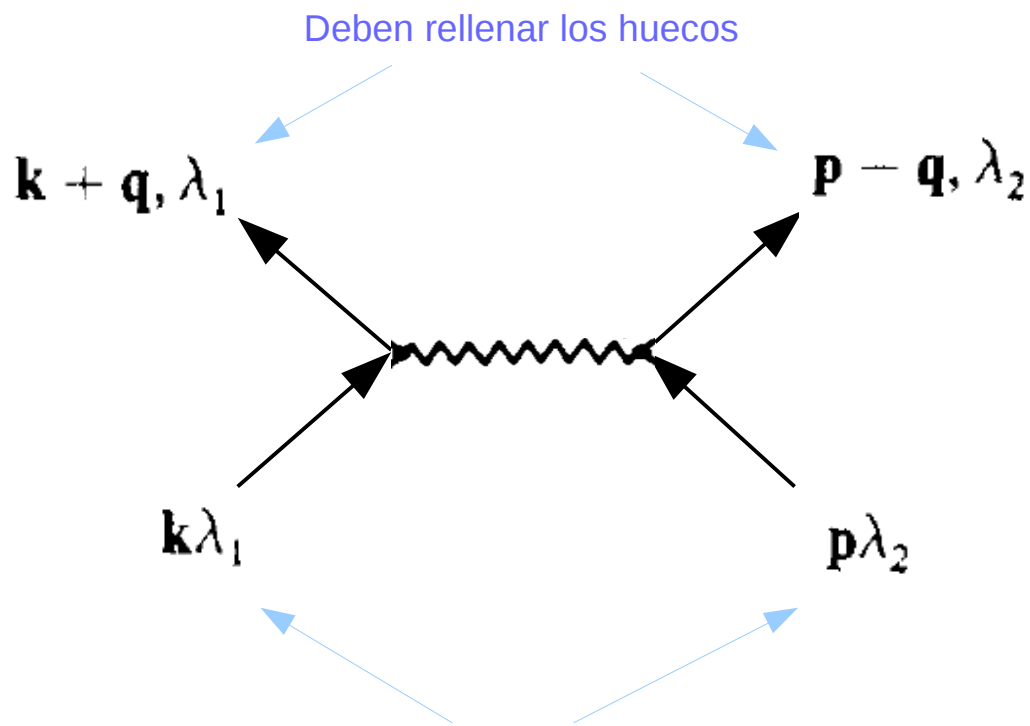
$$E^{(0)}/N = \frac{3 \hbar^2 k_F^2}{5 \cdot 2m}$$

$$\epsilon_F^0 = \hbar^2 k_F^2 / 2m \quad \text{Energía de Fermi}$$

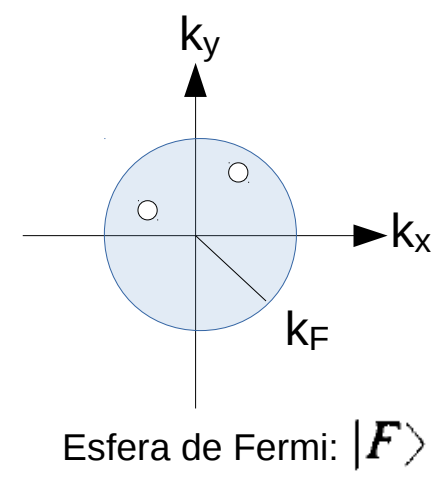
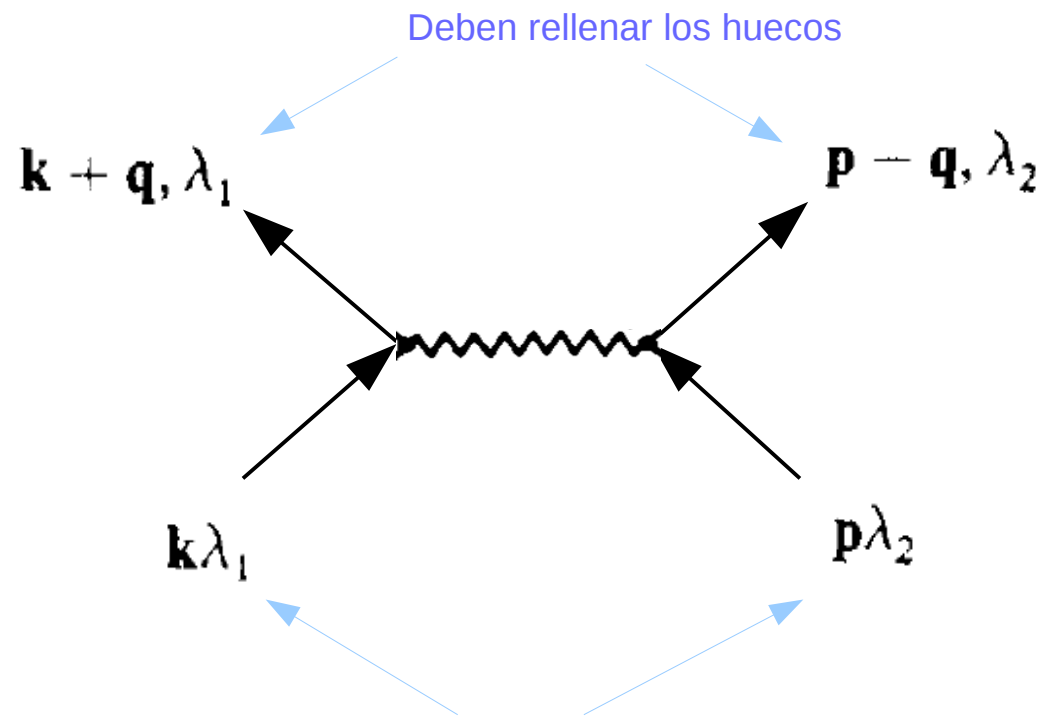
# Gas de electrones: Jellium model

Corrección a primer orden de la energía:

$$E^{(1)} = \langle F | \hat{H}_1 | F \rangle$$
$$= \frac{e^2}{2V} \sum_{\mathbf{k} \neq \mathbf{q}} \sum_{\lambda_1 \lambda_2} \frac{4\pi}{q^2} \langle F | a_{\mathbf{k}+\mathbf{q}, \lambda_1}^\dagger a_{\mathbf{p}-\mathbf{q}, \lambda_2}^\dagger a_{\mathbf{p}\lambda_2} a_{\mathbf{k}\lambda_1} | F \rangle$$



# Gas de electrones: Jellium model



Deben estar ocupados para que los dos operadores de destrucción no den cero

Hay dos posibilidades:

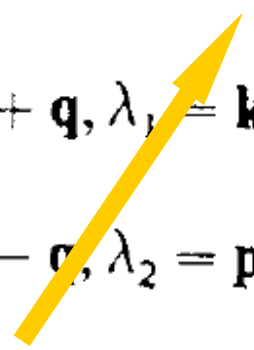
$\mathbf{q} \neq 0$

$\mathbf{k} + \mathbf{q}, \lambda_1 = \mathbf{k}\lambda_1$

$\mathbf{k} + \mathbf{q}, \lambda_1 = \mathbf{p}\lambda_2$

$\mathbf{p} - \mathbf{q}, \lambda_2 = \mathbf{p}\lambda_2$

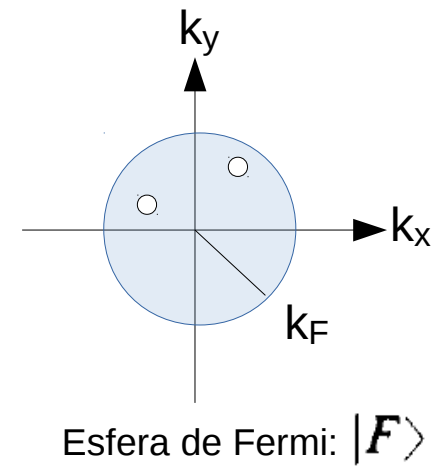
$\mathbf{p} - \mathbf{q}, \lambda_2 = \mathbf{k}\lambda_1$



# Gas de electrones: Jellium model

$$E^{(1)} = \langle F | \hat{H}_1 | F \rangle$$

$$= \frac{e^2}{2V} \sum_{\mathbf{k} \neq \mathbf{q}} \sum_{\lambda_1 \lambda_2} \frac{4\pi}{q^2} \langle F | a_{\mathbf{k}+\mathbf{q}, \lambda_1}^\dagger a_{\mathbf{p}-\mathbf{q}, \lambda_2}^\dagger a_{\mathbf{p} \lambda_2} a_{\mathbf{k} \lambda_1} | F \rangle$$



$$\mathbf{k} + \mathbf{q}, \lambda_1 = \mathbf{p} \lambda_2$$



eliminemos  $\mathbf{p}$

$$\mathbf{p} - \mathbf{q}, \lambda_2 = \mathbf{k} \lambda_1$$

Dar vuelta usando el anticonmutador y que  $q \neq 0$

$$\delta_{\mathbf{k}+\mathbf{q}, \mathbf{p}} \delta_{\lambda_1 \lambda_2} \langle F | a_{\mathbf{k}+\mathbf{q}, \lambda_1}^\dagger \overbrace{a_{\mathbf{k} \lambda_1}^\dagger a_{\mathbf{k}+\mathbf{q}, \lambda_1}} a_{\mathbf{k} \lambda_1} | F \rangle$$

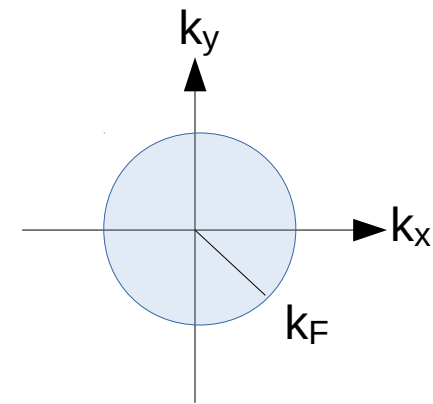
$$= -\delta_{\mathbf{k}+\mathbf{q}, \mathbf{p}} \delta_{\lambda_1 \lambda_2} \langle F | \hat{n}_{\mathbf{k}+\mathbf{q}, \lambda_1} \hat{n}_{\mathbf{k} \lambda_1} | F \rangle$$

$$= -\delta_{\mathbf{k}+\mathbf{q}, \mathbf{p}} \delta_{\lambda_1 \lambda_2} \theta(k_F - |\mathbf{k} + \mathbf{q}|) \theta(k_F - k)$$

# Gas de electrones: Jellium model

Usando las dos expresiones anteriores:

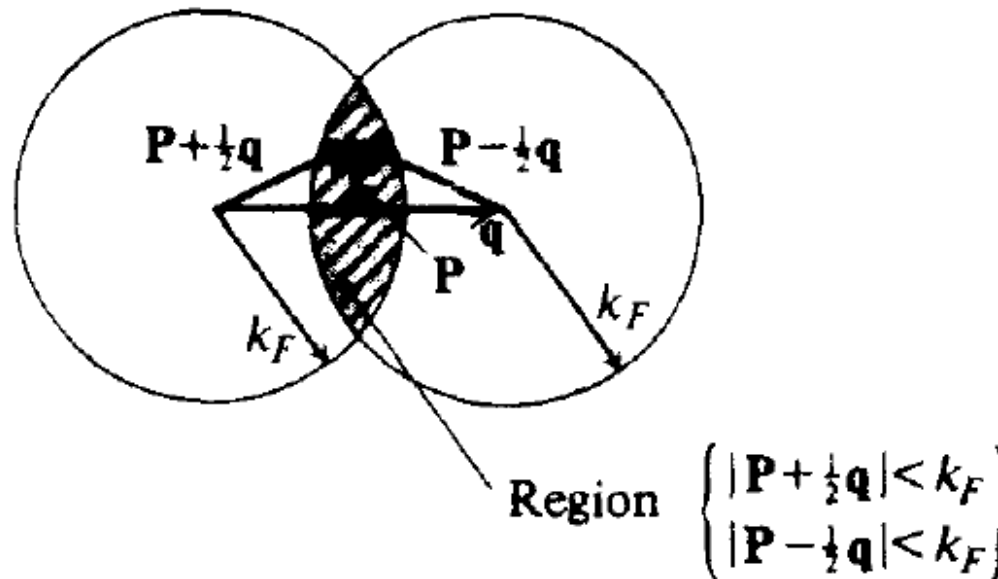
$$\begin{aligned}
 E^{(1)} &= -\frac{e^2}{2V} \sum_{\lambda_1} \sum_{\mathbf{k}\mathbf{q}} \frac{4\pi}{q^2} \theta(k_F - |\mathbf{k} + \mathbf{q}|) \theta(k_F - k) \\
 &= -\frac{e^2}{2} \frac{4\pi V}{(2\pi)^6} 2 \int d^3k d^3q q^{-2} \theta(k_F - |\mathbf{k} + \mathbf{q}|) \theta(k_F - k)
 \end{aligned}$$



Esfera de Fermi:  $|F\rangle$

Cambio de variable: from  $\mathbf{k}$  to  $\mathbf{P} = \mathbf{k} + \frac{1}{2}\mathbf{q}$   $\longrightarrow$

$$E^{(1)} = -4\pi e^2 V (2\pi)^{-6} \int d^3q q^{-2} \int d^3P \theta(k_F - |\mathbf{P} + \frac{1}{2}\mathbf{q}|) \theta(k_F - |\mathbf{P} - \frac{1}{2}\mathbf{q}|)$$

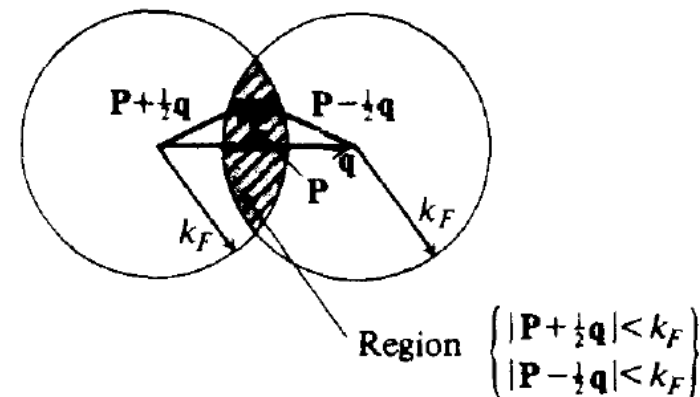




# Gas de electrones: Jellium model

$$E^{(1)} = -4\pi e^2 V (2\pi)^{-6} \int d^3q q^{-2} \int d^3P \theta(k_F - |\mathbf{P} + \frac{1}{2}\mathbf{q}|) \theta(k_F - |\mathbf{P} - \frac{1}{2}\mathbf{q}|)$$

Hay que calcular ese volumen, de la intersección de dos esferas con  $x \equiv \frac{q}{2k_F}$  se obtiene:



$$\int d^3P \theta(k_F - |\mathbf{P} + \frac{1}{2}\mathbf{q}|) \theta(k_F - |\mathbf{P} - \frac{1}{2}\mathbf{q}|) = \frac{4\pi}{3} k_F^3 (1 - \frac{3}{2}x + \frac{1}{2}x^3) \theta(1 - x)$$

$$\begin{aligned} \longrightarrow E^{(1)} &= -4\pi e^2 V (2\pi)^{-6} \frac{4\pi}{3} k_F^3 2k_F \int_0^1 dx 4\pi (1 - \frac{3}{2}x + \frac{1}{2}x^3) \\ &= -\frac{e^2}{2a_0} \frac{N}{r_s} \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{3}{2\pi} = -\frac{e^2}{2a_0} N \frac{0.916}{r_s} \end{aligned}$$

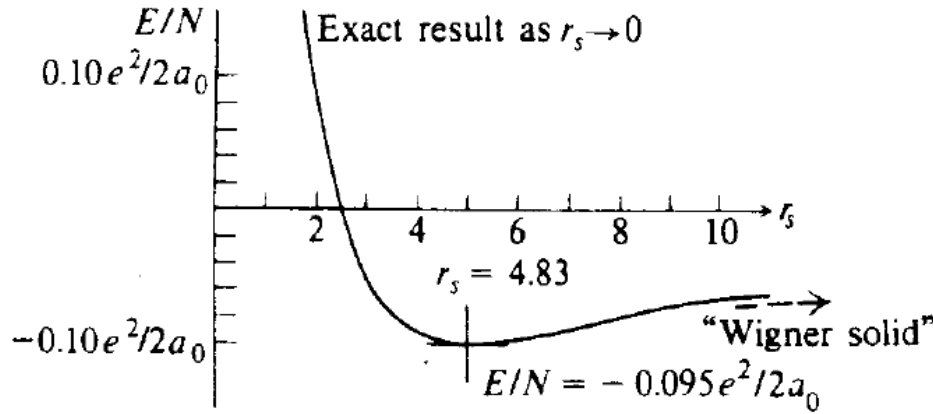
# Gas de electrones: Jellium model

Juntando las dos contribuciones:

$$\longrightarrow \frac{E}{N} \underset{r_s \rightarrow 0}{=} \frac{e^2}{2a_0} \left[ \frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \dots \right]$$

Energía cinética      Energía de intercambio      Energía de correlación ...

A primer orden en la energía Coulombiana (electrón-electrón) hay dos términos, el **directo** que corresponde a  $q=0$  y que se canceló con  $H_b + H_{el-b}$ , y el de **intercambio**, (exchange energy) que es negativo.



**Fig. 3.2** Approximate ground-state energy [first two terms in Eq. (3.37)] of an electron gas in a uniform positive background.

# Gas de electrones: Jellium model

1) Energías negativas indican que el GS es estable.

2) La energía exacta siempre será menor que la que obtuvimos nosotros “ensanguchando” con un estado que no es el verdadero GS.

3) El mínimo de energía está en:  $(r_s)_{\min} = 4.83$   $\left(\frac{E}{N}\right)_{\min} = -0.095 \frac{e^2}{2a_0} = -1.29 \text{ eV}$

Que está bastante bien comparado con:

$$r_s = 3.96 \quad \frac{E}{N} = -1.13 \text{ eV} \quad \text{Na (experiment)}$$

4) Podemos calcular la presión y la compresibilidad:

$$P = -\left(\frac{\partial E}{\partial V}\right)_N = -\frac{dE}{dr_s} \frac{dr_s}{dV} = \frac{Ne^2}{2a_0} \frac{r_s}{3V} \left[ \frac{2(2.21)}{r_s^3} - \frac{0.916}{r_s^2} \right]$$

$$B = -V \left(\frac{\partial P}{\partial V}\right)_N = \frac{Ne^2}{2a_0} \frac{2}{9V} \left[ \frac{5(2.21)}{r_s^2} - \frac{2(0.916)}{r_s} \right]$$

Se anula en:  
 $r_s = 4.83$

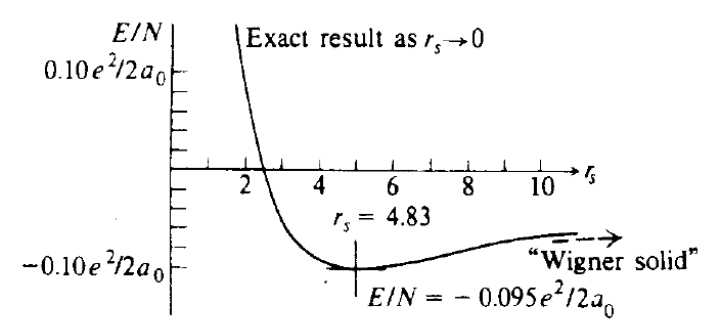


Fig. 3.2 Approximate ground-state energy [first two terms in Eq. (3.37)] of an electron gas in a uniform positive background.

# Gas de electrones: Jellium model

Yendo a densidades muy bajas ( $r_s$  grande) domina la interacción Coulombiana y pasa algo interesante:

## Transición a un **Cristal de Wigner**

**Los electrones se quedan localizados en los sitios de una red cristalina.**

La energía por partícula fue calculada por Wigner:

$$\frac{E}{N} \underset{r_s \rightarrow \infty}{=} \frac{e^2}{2a_0} \left[ -\frac{1.79}{r_s} + \frac{2.66}{r_s^{\frac{3}{2}}} + \dots \right] \quad \text{“Wigner solid”}$$

Y efectivamente es menor que la que obtuvimos antes.

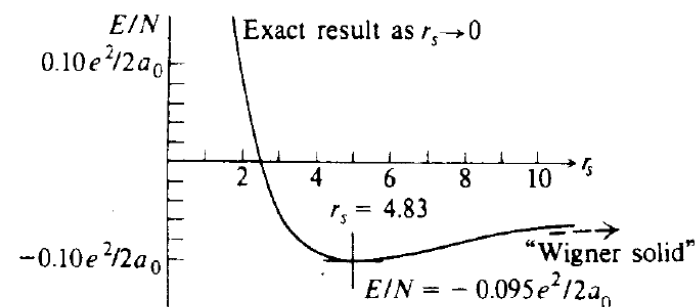


Fig. 3.2 Approximate ground-state energy [first two terms in Eq. (3.37)] of an electron gas in a uniform positive background.

<sup>4</sup> E. P. Wigner, *Trans. Farad. Soc.*, **34**:678 (1938); W. J. Carr, Jr., *Phys. Rev.*, **122**:1437 (1961).

# Jellium model: ejercicio

2. (a) Escribir en segunda cuantización el Hamiltoniano de un gas de electrones quasi-bidimensional, cuyo Hamiltoniano en primera cuantización es:

$$H^{(1)} = \sum_{i=1}^N \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{i=1}^N u(z_i) \quad (1)$$

Sugerencia: Utilizar como base de partícula única los estados:

$$\psi_{n\mathbf{k}\sigma}(\mathbf{r}, s) = \frac{1}{L} e^{i\mathbf{k} \cdot \boldsymbol{\rho}} \varphi_n(z) \chi_\sigma(s) \quad (2)$$

donde  $\mathbf{k} = (k_x, k_y)$ ,  $\boldsymbol{\rho} = (x, y)$  y  $\varphi_n(z)$  satisface:

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + u(z) \right] \varphi_n(z) = \varepsilon_n \varphi_n(z) \quad (3)$$

Ayuda:

$$\int d^2\rho \frac{e^{i\mathbf{q} \cdot \boldsymbol{\rho}}}{\sqrt{\rho^2 + (z - z')^2}} = \int_0^\infty d\rho \int_0^{2\pi} d\phi \frac{\rho e^{iq\rho \cos \phi}}{\sqrt{\rho^2 + (z - z')^2}} \quad (4)$$

$$= 2\pi \int_0^\infty d\rho \frac{\rho J_0(q\rho)}{\sqrt{\rho^2 + (z - z')^2}} = \frac{2\pi}{q} e^{-q|z - z'|} \quad (5)$$

- (b) Escribir en segunda cuantización el Hamiltoniano para el jellium model en dos dimensiones (obtener una expresión equivalente la Ec. (3.19) de Fetter-Walecka).