FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

1º Semestre de 2023

02/08/2023

Aula 2

O gás uniforme de elétrons ("jellium model")

SISTEMA FICTÍCIO DE UM GÁS DE ELÉTRONS NUMA "MATRIZ" UNIFORME POSITIVA (DE TAL FORMA A CANCELAR A CARGA ELÉTRICA). O QUE CARACTERIZA O SISTEMA:

a) DENSIDADE: $\underline{N}$ ELÉTRONS, NUMA CAIXA DE VOLUME $\underline{V}$

$$n = \frac{N}{V}$$

LIMITE TERMODINÂMICO: $N \to \infty$, $V \to \infty$, $n = \text{CONST.}$

b) TEMPERATURA: VAMOS FOCAR NO EST. FUND. ($T = 0$)

TOMAREMOS A INTERAÇÃO COMO SENDO:

$$V(\vec{r}) = \pm \frac{e^2}{r} e^{-\mu r}$$

NO FIM, TOMAMOS $\mu \to 0$

SE $\mu = 0$ DESDE O INÍCIO, O CARÁTER DE LONGO ALCANCE DA INTERAÇÃO COULOMBIANA APRESENTA DIFICULDADES. (CF. COM A CONSTRUÇÃO DE EWALD DO ESTADO SÓLIDO).

MATRIZ POSITIVA UNIFORME COM DENSIDADE DE CARGA:

$$\rho_p = ne$$

$$Q_p = \int \rho_p \, dV = Ne = -\text{CARGA TOTAL DOS ELÉTRONS.}$$

O Hamiltoniano na base de posição

$$H_{EG} = K_e + U_{ee} + U_{pp} + U_{ep}$$

$$K = \sum_{\sigma} \int d^3 r \psi_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \psi_{\sigma}(\mathbf{r})$$

$$U_{ee} = \frac{e^2}{2} \sum_{\sigma\sigma'} \int d^3 r d^3 r' \frac{e^{-\mu|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma'}^{\dagger}(\mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \psi_{\sigma}(\mathbf{r})$$

$$U_{pp} = \frac{\rho^2}{2} \int d^3 r_1 d^3 r_2 \frac{e^{-\mu|\mathbf{r}_1-\mathbf{r}_2|}}{|\mathbf{r}_1-\mathbf{r}_2|}$$

$\rho = ne$

$$U_{ep} = -\rho e \sum_{\sigma} \int d^3 r_1 d^3 r \frac{e^{-\mu|\mathbf{r}_1-\mathbf{r}|}}{|\mathbf{r}_1-\mathbf{r}|} \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r})$$

Análise de U_{pp} e U_{ep}

$$U_{pp} = \frac{\rho^2}{2}\int d^3r_1 d^3r_2 \frac{e^{-\mu|\mathbf{r}_1-\mathbf{r}_2|}}{|\mathbf{r}_1-\mathbf{r}_2|}$$

$$= \frac{e^2}{2}\left(\frac{N}{V}\right)^2 \underbrace{\int d^3r_1}_{V} \underbrace{d^3x \frac{e^{-\mu x}}{x}}_{U(0)}$$

$$\vec{x} = \vec{r}_1 - \vec{r}_2 \qquad \left.\begin{matrix}\vec{r}_1 \\ \vec{r}_2\end{matrix}\right\} \to \left\{\begin{matrix}\vec{r}_1 \\ \vec{x}\end{matrix}\right.$$

$$d^3r_1 d^3r_2 \Rightarrow d^3r_1 d^3x$$

DEFINO: TR. FOURIER: $U(\vec{q}) = \int d^3x\, e^{-i\vec{q}\cdot\vec{x}} \frac{e^{-\mu x}}{x} =$

$$= \int d^3x\, e^{-iqx\cos\theta} \frac{e^{-\mu x}}{x} = \int_0^\infty x^2 dx \int_0^\pi 2\pi \sin\theta\, d\theta\, e^{-iqx\cos\theta} \frac{e^{-\mu x}}{x}$$

$$= \frac{4\pi}{q^2+\mu^2} \Rightarrow U(0) = \frac{4\pi}{\mu^2}$$

$$\boxed{U_{pp} = \frac{e^2}{2}\frac{N^2}{V}\frac{4\pi}{\mu^2}}$$

$$U_{ep} = -\rho e \sum_{\sigma} \int d^3r_1 d^3r \frac{e^{-\mu|\mathbf{r}_1-\mathbf{r}|}}{|\mathbf{r}_1-\mathbf{r}|} \psi^\dagger_\sigma(\mathbf{r})\psi_\sigma(\mathbf{r})$$

$$\vec{x} = \vec{r}_1 - \vec{r}$$

$$= -\frac{N}{V} e^2 \sum_\sigma \int d^3r \, \underbrace{d^3x \frac{e^{-\mu x}}{x}}_{v(0)} \psi^\dagger_\sigma(\vec{r})\psi_\sigma(\vec{r})$$

$$= -\frac{N}{V} e^2 v(0) \underbrace{\sum_\sigma \int d^3r \, \psi^\dagger_\sigma(\vec{r})\psi_\sigma(\vec{r})}_{\hat{N} \to N} = -\frac{N^2}{V} e^2 \frac{4\pi}{\mu^2}$$

$$\boxed{U_{pp} + U_{ep} = -\frac{N^2}{2V} \frac{4\pi e^2}{\mu^2}}$$

K_e na base de momentos

BASE DE ESTADOS DE PARTÍCULA ÚNICA:

$$\langle \vec{r} | \vec{k} \rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \qquad \int d^3r \, |\psi_{\vec{k}}(\vec{r})|^2 = \int d^3r \, \frac{1}{V} = 1$$

$$K_e = \sum_\sigma \int d^3r \, \psi_\sigma^\dagger(\vec{r}) \left[-\frac{\nabla^2}{2m} \right] \psi_\sigma(\vec{r})$$ (BASE DE POSIÇÃO)

$$= \sum_\sigma \sum_{\vec{k}} \left(\frac{k^2}{2m} \right) a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}$$ (BASE DE MOMENTOS $\vec{k}\rangle$

$$K_e = \sum_{\vec{k}\sigma} \left(\frac{k^2}{2m} \right) \underbrace{a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}}_{\hat{n}_{\vec{k}\sigma}}$$

$$\psi_\sigma^\dagger(\vec{r}) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} a^\dagger_{\vec{k}\sigma}$$

$$U_{ee} = \frac{e^2}{2}\sum_{\sigma\sigma'}\int d^3r d^3r' \frac{e^{-\mu|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\psi_\sigma^\dagger(\mathbf{r})\,\psi_{\sigma'}^\dagger(\mathbf{r}')\,\psi_{\sigma'}(\mathbf{r}')\,\psi_\sigma(\mathbf{r})$$

$$= \frac{1}{2}\sum_{\substack{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4\\ \sigma_1,\sigma_2,\sigma_3,\sigma_4}} \underbrace{\langle \vec{k}_1\sigma_1;\vec{k}_2\sigma_2|U|\vec{k}_3\sigma_3;\vec{k}_4\sigma_4\rangle}_{\Delta} a^+_{\vec{k}_1\sigma_1} a^+_{\vec{k}_2\sigma_2} a_{\vec{k}_4\sigma_4} a_{\vec{k}_3\sigma_3}$$

$$\Delta = \langle\sigma_1,\sigma_2|\sigma_3,\sigma_4\rangle \int\frac{d^3r_1\, d^3r_2}{V^2} e^{-i\vec{k}_1\cdot\vec{r}_1} e^{-i\vec{k}_2\cdot\vec{r}_2}\left[\frac{e^2 e^{-\mu|\vec{r}_1-\vec{r}_2|}}{|\vec{r}_1-\vec{r}_2|}\right]\times$$

$$\times e^{i\vec{k}_3\cdot\vec{r}_1} e^{i\vec{k}_4\cdot\vec{r}_2} = \delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\frac{e^2}{V^2}\int d^3r_1 d^3r_2\, e^{-i[(\vec{k}_1-\vec{k}_3)\cdot\vec{r}_1+(\vec{k}_2-\vec{k}_4)\cdot\vec{r}_2]}$$

$$\times\frac{e^{-\mu|\vec{r}_1-\vec{r}_2|}}{|\vec{r}_1-\vec{r}_2|}$$

$$\vec{x} = \vec{r}_1-\vec{r}_2 \Rightarrow \vec{r}_2 = \vec{r}_1-\vec{x}$$

$$= \frac{e^2}{V^2}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\int d^3r_1 d^3x\, e^{-i[(\vec{k}_1-\vec{k}_3+\vec{k}_2-\vec{k}_4)\cdot\vec{r}_1]} e^{i(\vec{k}_2-\vec{k}_4)\cdot\vec{x}}\times$$

$$\times\frac{e^{-\mu x}}{x}$$

$$\int d^3x \, e^{-i\vec{q}\cdot\vec{x}} = \delta_{\vec{q},0} V$$

$$\rightarrow V \delta_{\vec{k}_1+\vec{k}_2,\vec{k}_3+\vec{k}_4}$$

$$\int d^3x \, e^{i(\vec{k}_2-\vec{k}_4)\cdot\vec{x}} \frac{e^{-\mu x}}{x} = U(\vec{k}_4-\vec{k}_2)$$

$$U_{ee} = \frac{e^2}{2V} \sum_{\substack{\vec{k}_1 \dots \\ \sigma_1 \dots}} \delta_{\sigma_1\sigma_3} \delta_{\sigma_2\sigma_4} \delta_{\vec{k}_1+\vec{k}_2,\vec{k}_3+\vec{k}_4} U(\vec{k}_4-\vec{k}_2) \times a^\dagger_{\vec{k}_1\sigma_1} a^\dagger_{\vec{k}_2\sigma_2} a_{\vec{k}_4\sigma_4} a_{\vec{k}_3\sigma_3}$$

$$= \frac{e^2}{2V} \sum_{\substack{\vec{k}_1 \dots \\ \sigma_1\sigma_2}} \delta_{\vec{k}_1+\vec{k}_2,\vec{k}_3+\vec{k}_4} U(\vec{k}_4-\vec{k}_2) a^\dagger_{\vec{k}_1\sigma_1} a^\dagger_{\vec{k}_2\sigma_2} a_{\vec{k}_4\sigma_2} a_{\vec{k}_3\sigma_1}$$

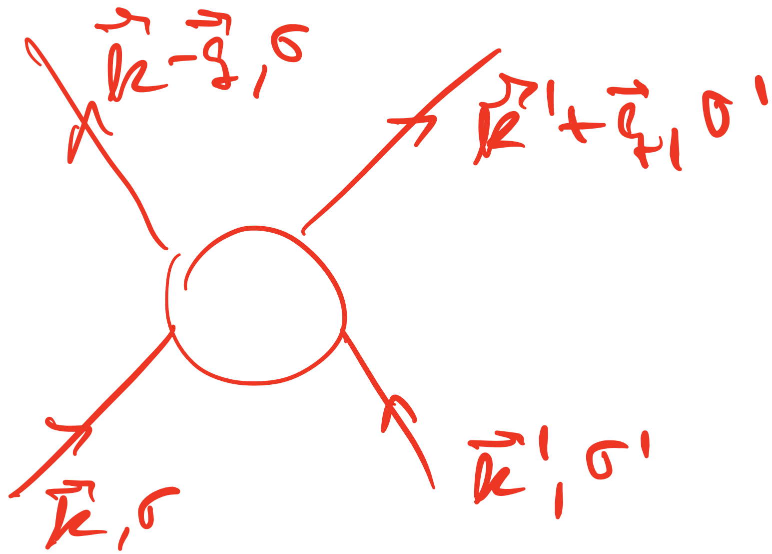
$$\vec{k}_1 = \vec{k}_3 - \vec{q}$$

$$\vec{k}_2 = \vec{k}_4 + \vec{q}$$

$$\vec{k}_4 - \vec{k}_2 = -\vec{q}$$

$$= \frac{e^2}{2V} \sum_{\substack{\vec{k}_3,\vec{k}_4,\vec{q} \\ \sigma_1,\sigma_2}} U(\vec{q}) a^\dagger_{\vec{k}_3-\vec{q},\sigma_1} a^\dagger_{\vec{k}_4+\vec{q},\sigma_2} a_{\vec{k}_4\sigma_2} a_{\vec{k}_3\sigma_1}$$

$$= \frac{e^2}{2V} \sum_{\substack{\vec{k},\vec{k}',\vec{q} \\ \sigma\sigma'}} U(\vec{q}) a^\dagger_{\vec{k}-\vec{q},\sigma} a^\dagger_{\vec{k}'-\vec{q},\sigma'} a_{\vec{k}',\sigma'} a_{\vec{k},\sigma}$$



$$U(\vec{q}) = \frac{4\pi}{q^2+\mu^2}$$

$$\{a_\lambda, a_\mu^\dagger\} = \delta_{\lambda\mu}$$

$$a_\lambda a_\mu^\dagger = -a_\mu^\dagger a_\lambda + \delta_{\lambda\mu}$$

TERMO $\vec{q}=0$ DE U_{ee}:

$$U_{ee}(\vec{q}=0) = \frac{e^2}{2V} \sum_{\substack{\vec{k},\vec{k}' \\ \sigma,\sigma'}} U(0)\, \underbrace{a^\dagger_{\vec{k},\sigma} a^\dagger_{\vec{k}',\sigma'} a_{\vec{k}',\sigma'} a_{\vec{k},\sigma}}$$

$$-a^\dagger_{\vec{k}\sigma} a^\dagger_{\vec{k}',\sigma'} a_{\vec{k},\sigma} a_{\vec{k}',\sigma'} =$$

$$= + a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma} a^\dagger_{\vec{k}',\sigma'} a_{\vec{k}',\sigma'} -$$

$$- \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'} a^\dagger_{\vec{k},\sigma} a_{\vec{k},\sigma} =$$

$$= \hat{n}_{\vec{k}\sigma} \hat{n}_{\vec{k}'\sigma'} - \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'} \hat{n}_{\vec{k},\sigma}$$

$$U_{ee}(\vec{q}=0) = \frac{e^2}{2V} U(0) \sum_{\substack{\vec{k}\vec{k}' \\ \sigma\sigma'}} \left[\hat{n}_{\vec{k},\sigma} \hat{n}_{\vec{k}',\sigma'} - \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'} \hat{n}_{\vec{k}\sigma} \right]$$

$$= \frac{e^2}{2V} U(0) \left[\underbrace{\left(\sum_{\vec{k},\sigma} \hat{n}_{\vec{k}\sigma} \right)}_{\hat{N}} \underbrace{\left(\sum_{\vec{k}'\sigma'} \hat{n}_{\vec{k}',\sigma'} \right)}_{\hat{N}} - \underbrace{\sum_{\vec{k},\sigma} \hat{n}_{\vec{k}\sigma}}_{\hat{N}} \right]$$

$$= \frac{e^2}{2V} U(0) \left(N^2 - N \right) = \frac{N^2 e^2}{2V} U(0) \left(1 - \cancel{\frac{1}{N}} \right) \quad \rightarrow 0$$

$$= \frac{N^2}{2V} e^2 \frac{4\pi}{\mu^2} = -\left(U_{pp} + U_{ep} \right)$$

$$U(\vec{q}) = \frac{4\pi}{q^2 + \mu^2} \xrightarrow[\mu \to 0]{} U(q) = \frac{4\pi}{q^2}$$

$$\sum_{\vec{k}} = \frac{V}{(2\pi)^3} \int d^3k$$

$$\vec{k} = (k_x, k_y, k_z) \xrightarrow{PBC} \frac{2\pi}{L} (n_x, n_y, n_z)$$

Gás uniforme de elétrons
("jellium model")

$$H_{EG} = \sum_{\mathbf{k},\sigma} \frac{k^2}{2m} a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \frac{1}{2V} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}\neq 0,\sigma_1,\sigma_2} \frac{4\pi e^2}{q^2} a^\dagger_{\mathbf{k}_1+\mathbf{q},\sigma_1} a^\dagger_{\mathbf{k}_2-\mathbf{q},\sigma_2} a_{\mathbf{k}_2,\sigma_2} a_{\mathbf{k}_1,\sigma_1}$$

Escala de comprimento disponível: raio de Bohr $a_0 = \frac{\hbar^2}{me^2}$

Escala de energia disponível: Rydberg $1 \text{ Ryd} = \frac{e^2}{2a_0} = 13.6 \text{ eV}$

$\vec{k} = a_0 \vec{k}'$, . . . $[\vec{k}'] = 1$

DISTÂNCIA MÉDIA ENTRE OS ELÉTRONS: $\frac{V}{N} = \frac{4\pi}{3}(r_s a_0)^3$

r_s: MEDIDA DO VOLUME/ELÉTRON

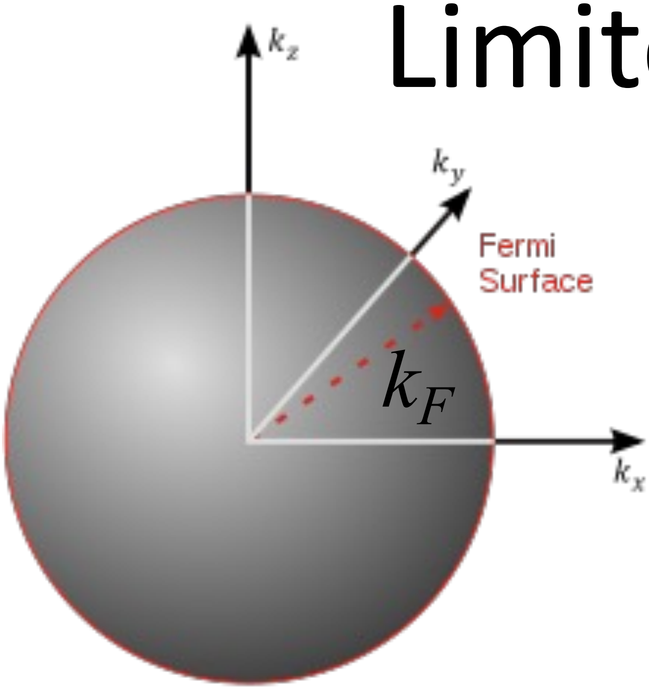
$r_s^3 \sim \frac{1}{n}$

r_s GRANDE = BAIXA DENSIDADE

r_s PEQUENO = ALTA DENSIDADE

$$H_{EG} = \frac{e^2}{a_0} \frac{1}{r_s^2} \left(\sum_{\mathbf{k}',\sigma} \frac{k'^2}{2} a^\dagger_{\mathbf{k}',\sigma} a_{\mathbf{k}',\sigma} + \frac{3r_s}{2N} \sum_{\mathbf{k}'_1,\mathbf{k}'_2,\mathbf{q}'\neq 0,\sigma_1,\sigma_2} \frac{1}{q'^2} a^\dagger_{\mathbf{k}'_1+\mathbf{q}',\sigma_1} a^\dagger_{\mathbf{k}'_2-\mathbf{q}',\sigma_2} a_{\mathbf{k}'_2,\sigma_2} a_{\mathbf{k}'_1,\sigma_1} \right)$$

Limite de alta densidade



$$n = \frac{k_F^3}{3\pi^2}$$

$$k_F = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_s a_0}$$

$$N = \sum_{\vec{k}\sigma} n_{\vec{k},\sigma} = \sum_{\vec{k},\sigma} \theta(k_F - k) = 2\, V \int \frac{d^3k}{(2\pi)^3} \theta(k_F - k)$$

$$= \frac{2V}{(2\pi)^3} \frac{4}{3} \pi k_F^3 \Rightarrow \boxed{n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}}$$

$$E(r_s = 0) = \langle K_e \rangle = 2\, V \int \frac{d^3k}{(2\pi)^3} \theta(k_F - k) \frac{k^2}{2m} = \frac{V}{2\pi^2 m} \frac{k_F^5}{5} = \frac{3}{5} N \underbrace{\frac{k_F^2}{2m}}_{E_F}$$

$$= \frac{3}{5} N E_F = \frac{3}{5} N \frac{\left(\frac{9\pi}{4}\right)^{2/3}}{r_s^2} \text{Ryd} = \frac{2.2099\, N}{r_s^2} \text{Ryd}$$

EM TEORIA DE PERTURBAÇÃO EM r_s:

$\langle \hat{V} \rangle_0 \longrightarrow$ EXERCÍCIO DA LISTA

$$\frac{\langle \hat{V}_0 \rangle}{N} = -\frac{3}{2\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s}\,Ryd = -\frac{0.9163}{r_s}\,Ryd$$

$$\frac{E^{(1)}(r_s)}{N} = \left[\frac{2.2099}{r_s^2} - \frac{0.9163}{r_s}\right]Ryd$$

$$= \frac{1}{r_s^2}\left[2.2099 - 0.9163\, r_s\right]Ryd$$

Expansão de alta densidade

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

Limite de baixa densidade

$$H_{EG} = \frac{e^2}{a_0}\frac{1}{r_s^2}\left(\sum_{\mathbf{k}',\sigma}\frac{k'^2}{2}a^\dagger_{\mathbf{k}',\sigma}a_{\mathbf{k}',\sigma} + \frac{3r_s}{2N}\sum_{\mathbf{k}'_1,\mathbf{k}'_2,\mathbf{q}'\neq 0,\sigma_1,\sigma_2}\frac{1}{q'^2}a^\dagger_{\mathbf{k}'_1+\mathbf{q}',\sigma_1}a^\dagger_{\mathbf{k}'_2-\mathbf{q}',\sigma_2}a_{\mathbf{k}'_2,\sigma_2}a_{\mathbf{k}'_1,\sigma_1}\right)$$

MINIMIZAR A INTERAÇÃO → CONJECTURA: CRISTAL

→ WIGNER CRYSTAL

Expansão de baixa densidade

$$\frac{U}{N} = -\frac{1.8}{r_s}\ \mathrm{Ry}\ \mathrm{(3D)}$$
$$\frac{U}{N} = -\frac{2.2}{r_s}\ \mathrm{Ry}\ \mathrm{(2D)}$$

Table 1.3. *Energies per electron of the classical Wigner crystal for different Bravais lattices in three and two dimensions.*

d	Lattice	$\frac{U}{N}\left(\frac{Ry}{r_s}\right)$
3	Simple Cubic	−1.760
3	Face Centered Cubic	−1.79175
3	Body Centered Cubic	−1.79186
3	Hexagonal Close Packed	−1.79168
2	Square	−2.2
2	Hexagonal	−2.212

Fônons

$$\frac{\Delta U}{N} \approx \begin{cases} \frac{2.66}{r_s^{\frac{3}{2}}}\mathrm{Ry}\ , & (3D - \mathrm{bcc}), \\ \frac{1.59}{r_s^{\frac{3}{2}}}\mathrm{Ry}\ , & (2D - \mathrm{hexagonal}). \end{cases}$$

Estado fundamental (T=0)

3D:

50(2) — 106(1) — r_s

Líquido de Fermi paramagnético

Líquido de Fermi parcialmente polarizado FM

Cristal de Wigner bcc AFM ou FM?? não há precisão suficiente…

F. H. Zong, C. Lin, and D. M. Ceperley, Phys. Rev. E **66**, 036703 (2002).

86.6(7) — r_s

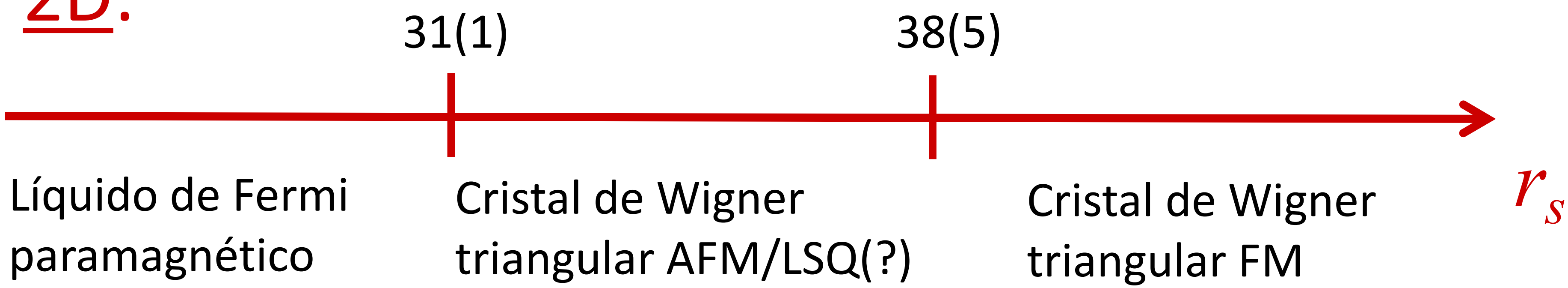
Líquido de Fermi paramagnético

Cristal de Wigner bcc AFM (?)

Sam Azadi and N. D. Drummond, PRB **105**, 245135 (2022).

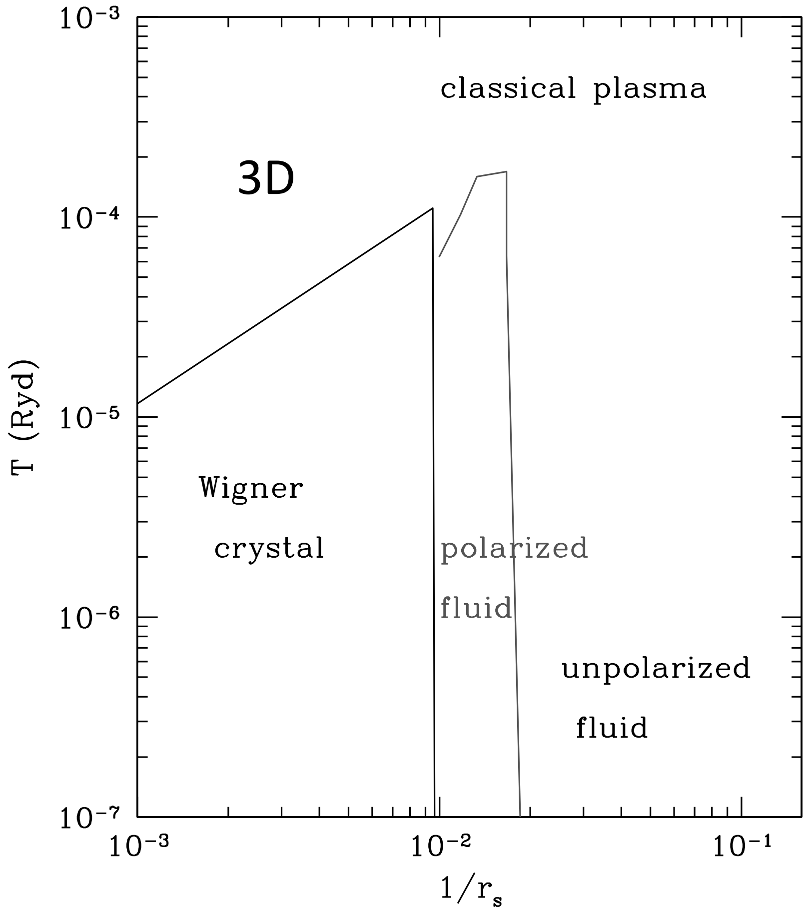
Estado fundamental (T=0)

2D:



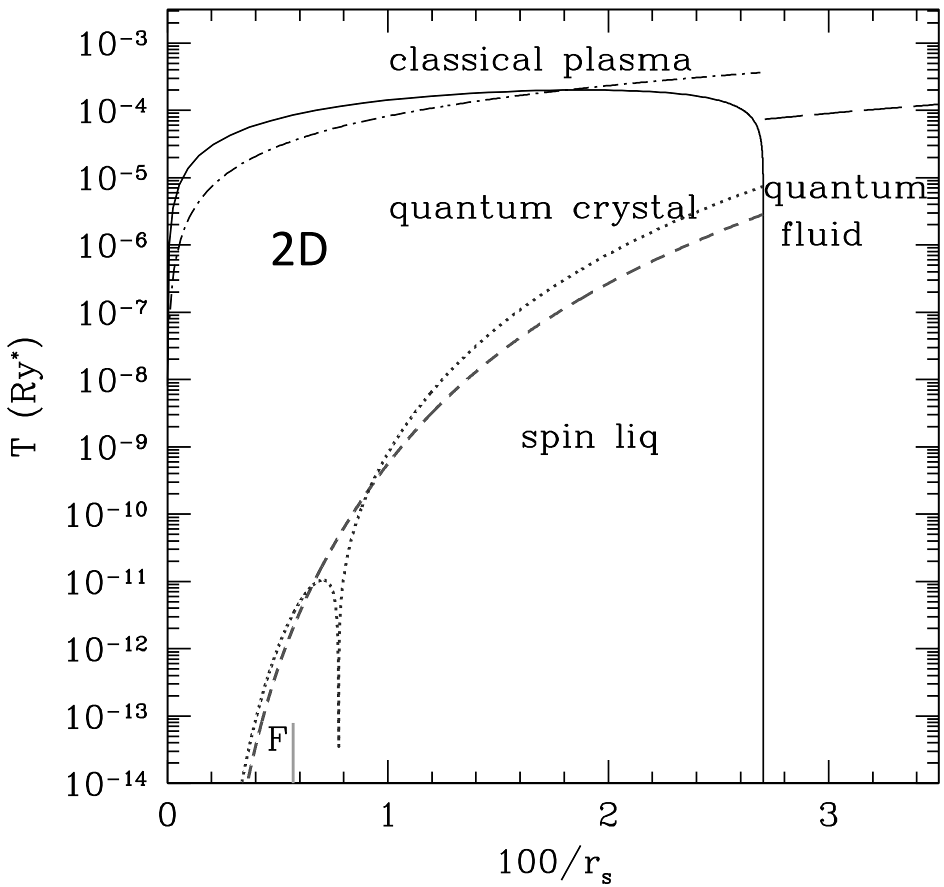
N. D. Drummond and R. J. Needs, PRL **102**, 126402 (2009)

Temperatura x densidade



Unp. liquid: $r_s < 50$
FM liquid: $50 < r_s < 100$
Wigner Crystal: $r_s > 100$

Ceperley, D. M. (2004). Introduction to quantum Monte Carlo methods applied to the electron gas, to appear in *The electron liquid paradigm in condensed matter physics*, Proceedings of the International School of Physics "Enrico Fermi", Course CLVII, edited by G. F. Giuliani and G. Vignale.



Unp. liquid: $r_s < 20$

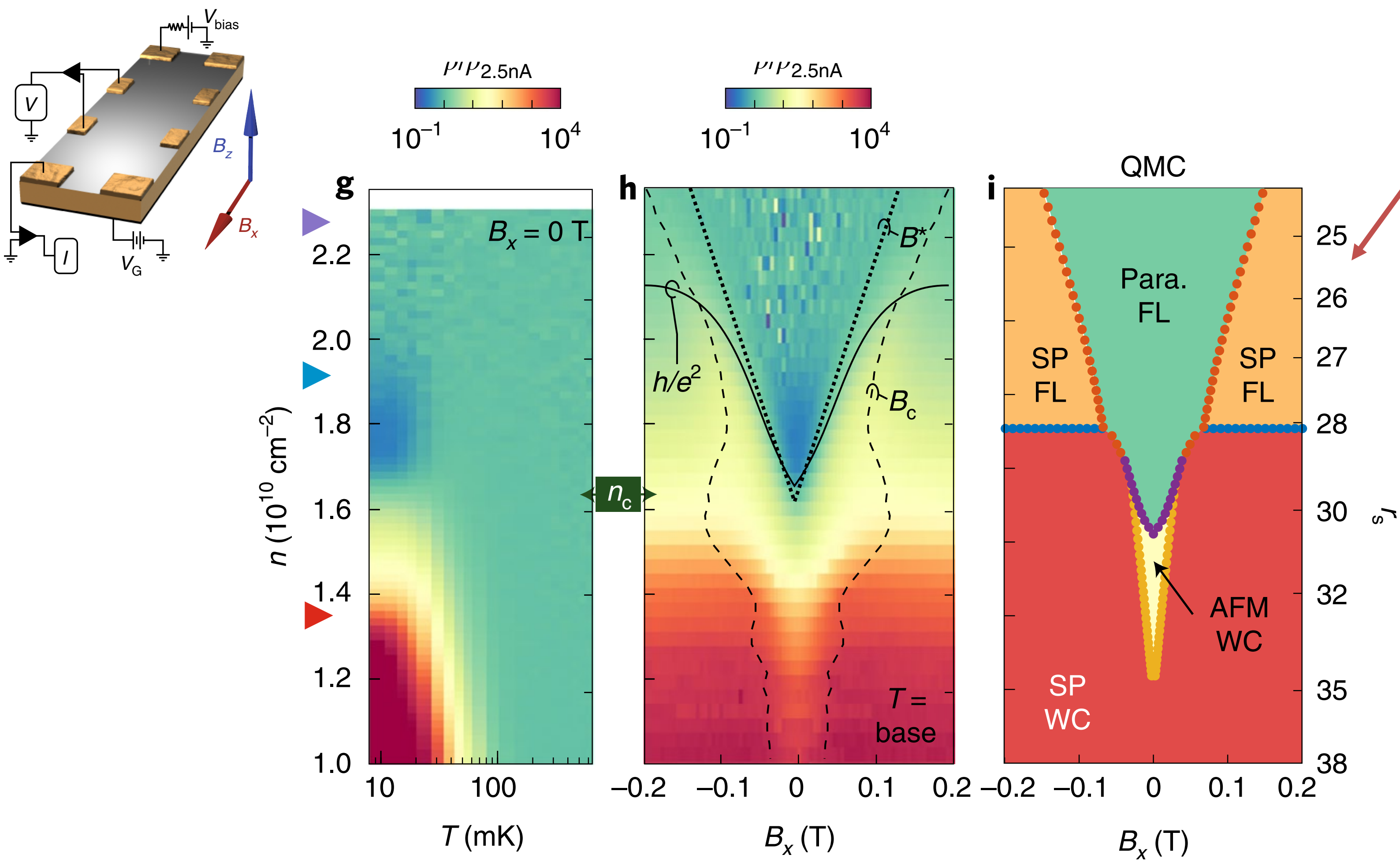
Wigner Crystal: $r_s > 34$

Bernu, B., Candido, L., and Ceperley, D. M. (2001). Exchange frequencies in the 2D Wigner crystal, *Physical Review Letters* **86**, 870–873.

Ref.: "Quantum theory of the electron liquid", Gabriele Giuliani and Giovanni Vignale, Cambridge (2005).

Resultados experimentais em 2D (ZnO)

“MgZnO/ZnO heterostructure confines a 2DES approximately 500 nm”



Drummond and Needs, PRL **102**, 126402 (2009)

J. Falson, I. Sodemann, B. Skinner, D. Tabrea, Y. Kozuka, A. Tsukazaki, M. Kawasaki, K. von Klitzing, and J. H. Smet, Nat. Mat. **21**, 311 (2022).