FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

2º Semestre de 2023
01/08/2023
Aula 1

http://sites.ifi.unicamp.br/emiranda/ (Aba Ensino)

Ementa (estimada) do curso:

- Alguns modelos comuns
- Teoria de perturbação
- Aplicações clássicas
- Resposta linear
- Supercondutividade

Avaliação: listas (50%) e monografia (50%)

Bibliografia: Notas de aula (serão postadas no site)
Mahan, Fetter & Walecka, Coleman

O problema de muitos corpos

CRISTAL: ÍONS E ELÉTRONS

PRIMEIRA ABORDAGEM: RESOLVER ($\hbar = 1 = k_B$)

$$H|\psi(t)\rangle = i\partial_t|\psi(t)\rangle$$ OU

$$H|\psi_E\rangle = E|\psi_E\rangle$$

PARA OS ELÉTRONS DADA A REDE DE ÍONS.

$\underline{\underline{N_e = 10^{23}}}$

$$H = \sum_{i=1}^{N_e} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i=1}^{N_e} V(\vec{r}_i) + \sum_{i<j} \underline{\underline{U(\vec{r}_i - \vec{r}_j)}}$$

$$U(\vec{r}) = \frac{e^2}{r}$$

$\psi(\vec{r}_1, \dots, \vec{r}_{N_e}) \rightarrow 3 \times N_e$ VARIÁVEIS

ABSOLUTAMENTE IMPOSSÍVEL DE SER RESOLVIDO NUMERICAMENTE, NEM A ARMAZENAGEM É POSSÍVEL

EXPERIMENTOS MEDEM QUANTIDADES MAIS SIMPLES, QUE REPRESENTAM MÉDIAS SOBRE OS ELÉTRONS, MÉDIAS TEMPORAIS, MÉDIAS ESPACIAIS, ETC.

A IDEIA É FOCAR EM OBJETOS MAIS SIMPLES:

(a) MATRIZ DENSIDADE DE UM CORPO:

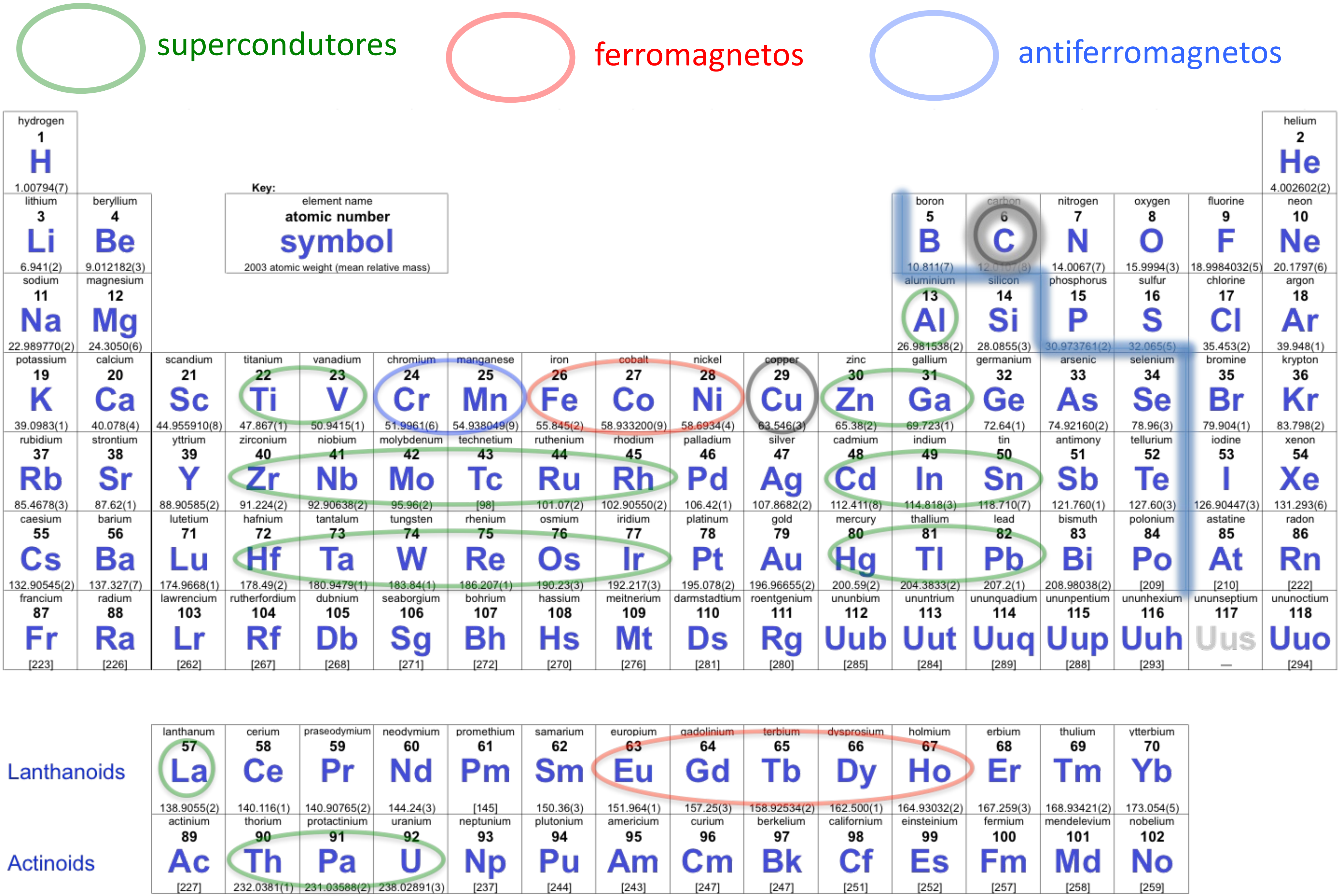
$$\rho(\vec{r}, \vec{r}\,') = \int d^3r_2\, d^3r_3 \cdots d^3r_{N_e}\, \psi^*(\vec{r}\,', \vec{r}_2, \vec{r}_3, \cdots, \vec{r}_N) \times$$

$$\times \psi(\vec{r}, \vec{r}_2, \vec{r}_3, \cdots, \vec{r}_N)$$

COM ELA É POSSÍVEL CALCULAR QUANTIDADES FÍSICAS, COMO QUALQUER VALOR ESPERADO DE UM OPERADOR DE UM CORPO.

(b) FUNÇÕES DE GREEN:

1 CORPO: $G(\vec{r}_1, t_1; \vec{r}_2, t_2) = -i \langle \Psi_{0H} | T[\psi_H(\vec{r}_1 t_1) \psi_H^\dagger(\vec{r}_2, t_2)] | \Psi_{0H}$



supercondutores

ferromagnetos

antiferromagnetos

Key:
element name
atomic number
symbol
2003 atomic weight (mean relative mass)

hydrogen **1** **H** 1.00794(7)																	helium **2** **He** 4.002602(2)
lithium **3** **Li** 6.941(2)	beryllium **4** **Be** 9.012182(3)											boron **5** **B** 10.811(7)	carbon **6** **C** 12.0107(8)	nitrogen **7** **N** 14.0067(7)	oxygen **8** **O** 15.9994(3)	fluorine **9** **F** 18.9984032(5)	neon **10** **Ne** 20.1797(6)
sodium **11** **Na** 22.989770(2)	magnesium **12** **Mg** 24.3050(6)											aluminium **13** **Al** 26.981538(2)	silicon **14** **Si** 28.0855(3)	phosphorus **15** **P** 30.973761(2)	sulfur **16** **S** 32.065(5)	chlorine **17** **Cl** 35.453(2)	argon **18** **Ar** 39.948(1)
potassium **19** **K** 39.0983(1)	calcium **20** **Ca** 40.078(4)	scandium **21** **Sc** 44.955910(8)	titanium **22** **Ti** 47.867(1)	vanadium **23** **V** 50.9415(1)	chromium **24** **Cr** 51.9961(6)	manganese **25** **Mn** 54.938049(9)	iron **26** **Fe** 55.845(2)	cobalt **27** **Co** 58.933200(9)	nickel **28** **Ni** 58.6934(4)	copper **29** **Cu** 63.546(3)	zinc **30** **Zn** 65.38(2)	gallium **31** **Ga** 69.723(1)	germanium **32** **Ge** 72.64(1)	arsenic **33** **As** 74.92160(2)	selenium **34** **Se** 78.96(3)	bromine **35** **Br** 79.904(1)	krypton **36** **Kr** 83.798(2)
rubidium **37** **Rb** 85.4678(3)	strontium **38** **Sr** 87.62(1)	yttrium **39** **Y** 88.90585(2)	zirconium **40** **Zr** 91.224(2)	niobium **41** **Nb** 92.90638(2)	molybdenum **42** **Mo** 95.96(2)	technetium **43** **Tc** [98]	ruthenium **44** **Ru** 101.07(2)	rhodium **45** **Rh** 102.90550(2)	palladium **46** **Pd** 106.42(1)	silver **47** **Ag** 107.8682(2)	cadmium **48** **Cd** 112.411(8)	indium **49** **In** 114.818(3)	tin **50** **Sn** 118.710(7)	antimony **51** **Sb** 121.760(1)	tellurium **52** **Te** 127.60(3)	iodine **53** **I** 126.90447(3)	xenon **54** **Xe** 131.293(6)
caesium **55** **Cs** 132.90545(2)	barium **56** **Ba** 137.327(7)	lutetium **71** **Lu** 174.9668(1)	hafnium **72** **Hf** 178.49(2)	tantalum **73** **Ta** 180.9479(1)	tungsten **74** **W** 183.84(1)	rhenium **75** **Re** 186.207(1)	osmium **76** **Os** 190.23(3)	iridium **77** **Ir** 192.217(3)	platinum **78** **Pt** 195.078(2)	gold **79** **Au** 196.96655(2)	mercury **80** **Hg** 200.59(2)	thallium **81** **Tl** 204.3833(2)	lead **82** **Pb** 207.2(1)	bismuth **83** **Bi** 208.98038(2)	polonium **84** **Po** [209]	astatine **85** **At** [210]	radon **86** **Rn** [222]
francium **87** **Fr** [223]	radium **88** **Ra** [226]	lawrencium **103** **Lr** [262]	rutherfordium **104** **Rf** [267]	dubnium **105** **Db** [268]	seaborgium **106** **Sg** [271]	bohrium **107** **Bh** [272]	hassium **108** **Hs** [270]	meitnerium **109** **Mt** [276]	darmstadtium **110** **Ds** [281]	roentgenium **111** **Rg** [280]	ununbium **112** **Uub** [285]	ununtrium **113** **Uut** [284]	ununquadium **114** **Uuq** [289]	ununpentium **115** **Uup** [288]	ununhexium **116** **Uuh** [293]	ununseptium **117** **Uus** —	ununoctium **118** **Uuo** [294]

Lanthanoids	lanthanum **57** **La** 138.9055(2)	cerium **58** **Ce** 140.116(1)	praseodymium **59** **Pr** 140.90765(2)	neodymium **60** **Nd** 144.24(3)	promethium **61** **Pm** [145]	samarium **62** **Sm** 150.36(3)	europium **63** **Eu** 151.964(1)	gadolinium **64** **Gd** 157.25(3)	terbium **65** **Tb** 158.92534(2)	dysprosium **66** **Dy** 162.500(1)	holmium **67** **Ho** 164.93032(2)	erbium **68** **Er** 167.259(3)	thulium **69** **Tm** 168.93421(2)	ytterbium **70** **Yb** 173.054(5)
Actinoids	actinium **89** **Ac** [227]	thorium **90** **Th** 232.0381(1)	protactinium **91** **Pa** 231.03588(2)	uranium **92** **U** 238.02891(3)	neptunium **93** **Np** [237]	plutonium **94** **Pu** [244]	americium **95** **Am** [243]	curium **96** **Cm** [247]	berkelium **97** **Bk** [247]	californium **98** **Cf** [251]	einsteinium **99** **Es** [252]	fermium **100** **Fm** [257]	mendelevium **101** **Md** [258]	nobelium **102** **No** [259]

Quebra espontânea de simetria

A emergência na física da matéria condensada e as quebras espontâneas de simetria, *Ciencia & Cultura* **65**, 32 (2013)

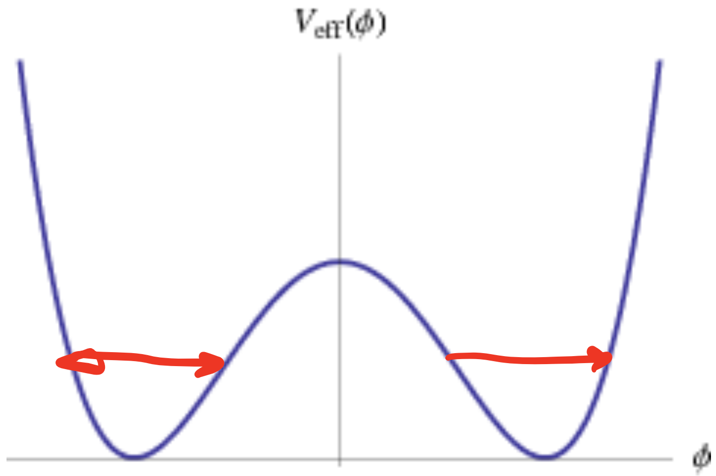
O ESTADO FUNDAMENTAL DE UM SISTEMA TEM MENOS SIMETRIA QUE O HAMILTONIANO.

FERROMAGNETO: $\vec{M} = \sum_i \langle \vec{S}_i \rangle \neq 0$ SE $T < T_c$

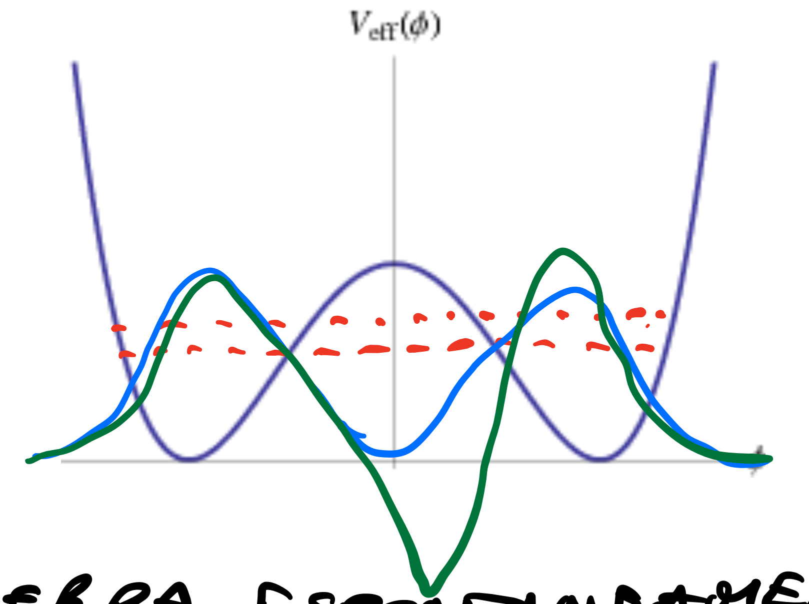
EMBORA H SEJA INVARIANTE POR ROTAÇÕES DE SPIN.

Comportamento clássico X quântico

Clássico



Quântico

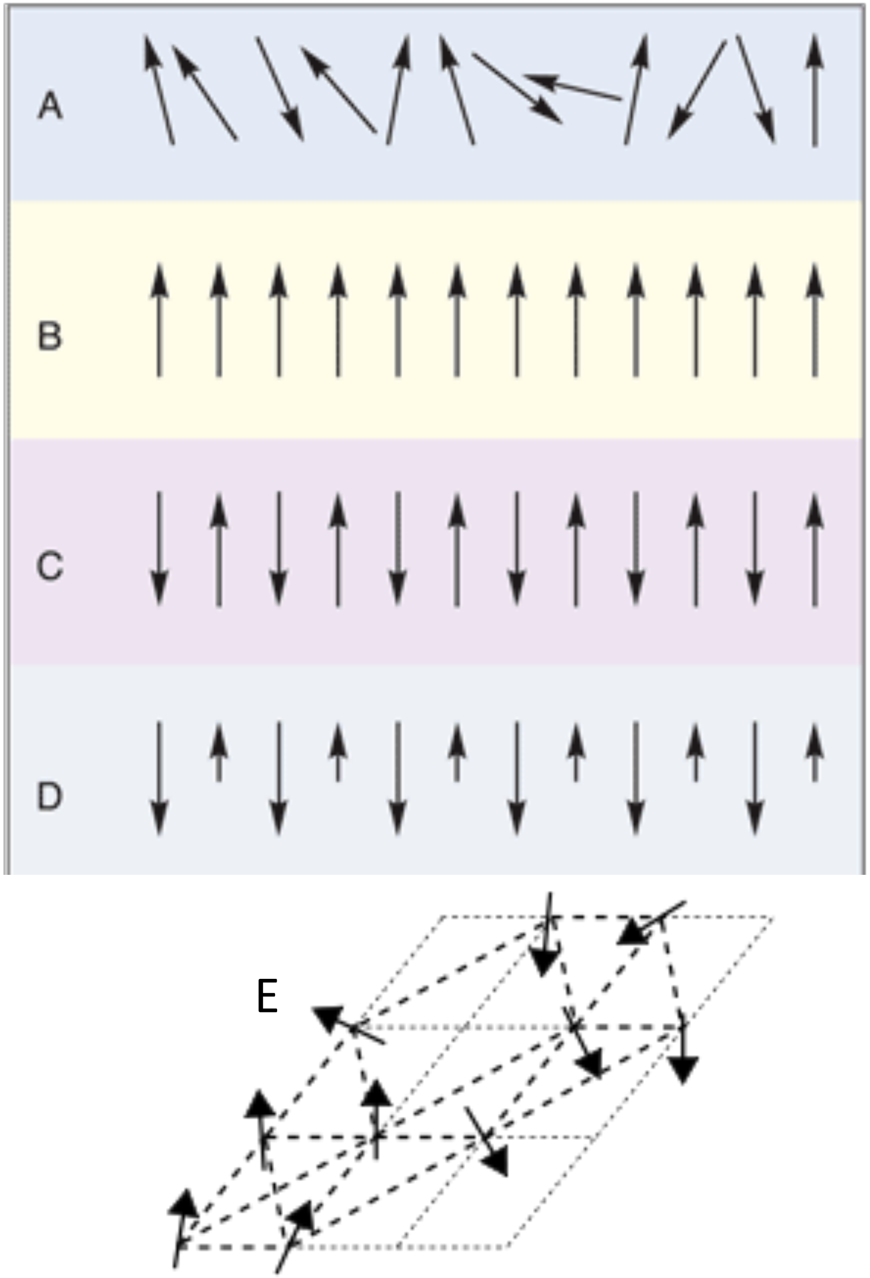


O SISTEMA CLÁSSICO QUEBRA ESPONTANEAMENTE A SIMETRIA $(\phi \to -\phi)$ DE $V(\phi)$ E DE H.

Ordem magnética

A. Paramagnetismo
B. Ferromagnetismo
C. Antiferromagnetismo
D. Ferrimagnetismo
E. Vidro de spin

Parâmetros de ordem

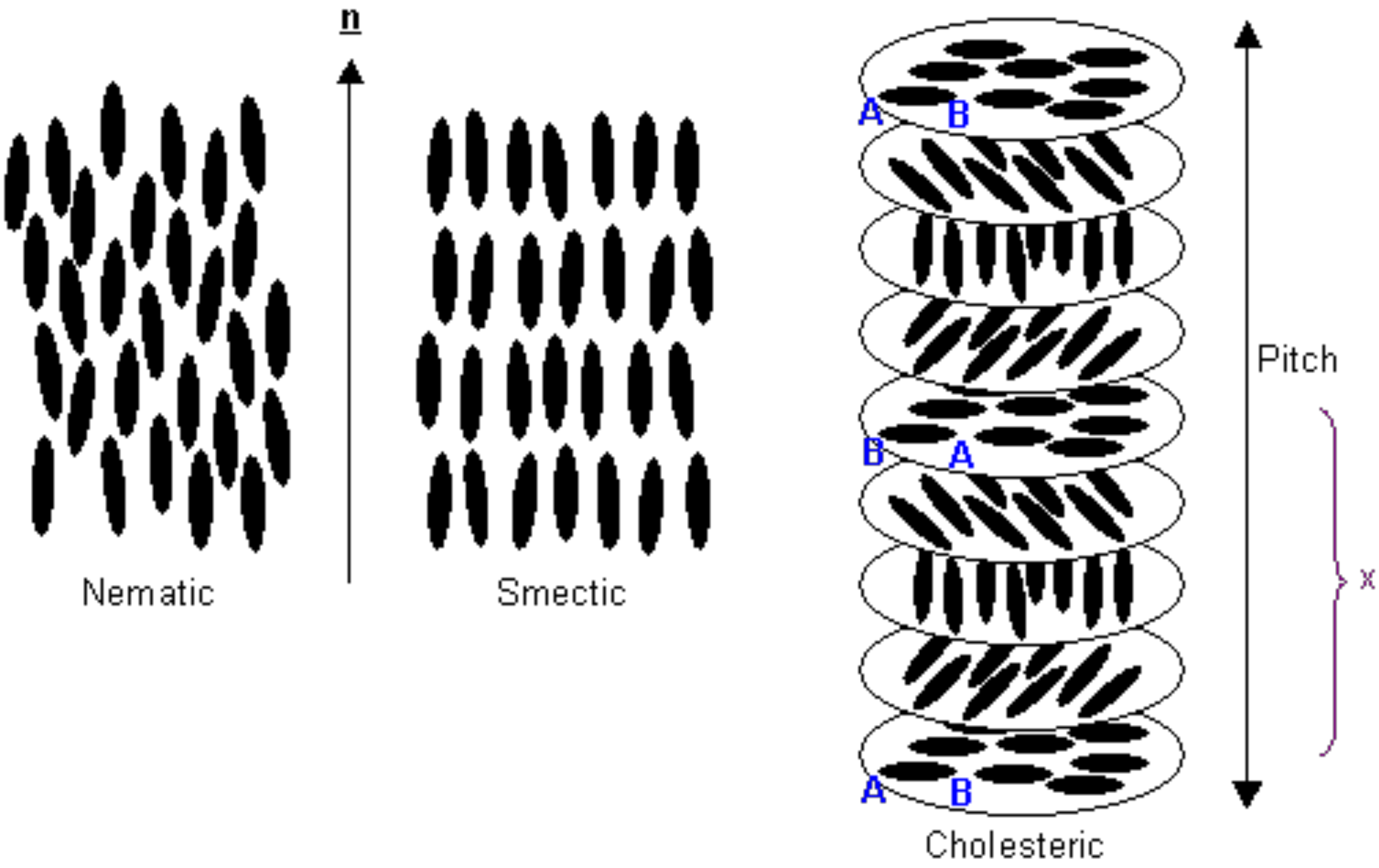


Ordem cristalina

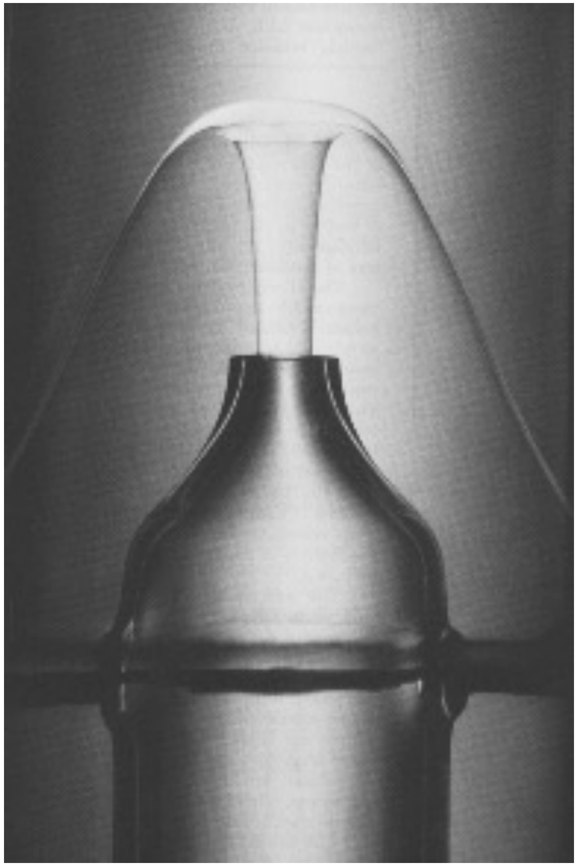
DENSIDADE $\rho(\vec{x})$:

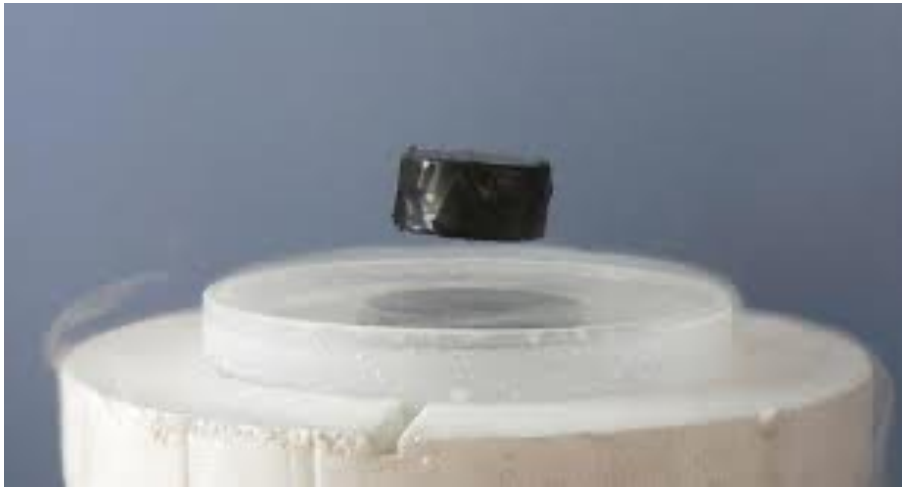
$$\tilde{\rho}(\vec{q}) = \int d^3x \, e^{i\vec{q}\cdot\vec{x}} \rho(\vec{x})$$

Cristais líquidos



Ordens superfluida e supercondutora





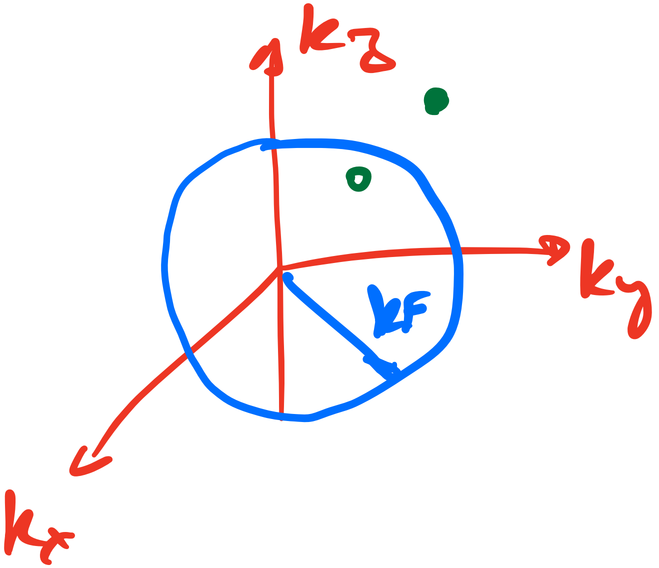
MATRIZ DENS. DE UM CORPO:

$$\rho(\vec{r},\vec{r}\,') \xrightarrow[|\vec{r}-\vec{r}\,'|\to\infty]{} \begin{cases} 0 & T > T_c \\ \text{CONST.} & T < T_c \end{cases}$$

Excitações elementares

DESCRIÇÃO DOS ESTADOS EXCITADOS DE UM SISTEMA: EXEMPLO: ELÉTRONS/FÉRMIONS

SEM INTERAÇÃO:



EST. FUND.: ESTADOS COM $k<k_F$ SÃO CHEIOS E TODOS COM $k>k_F$ SÃO VAZIOS

EXCITAÇÕES SÃO PARES ELÉTRON-BURACO

E COM INTERAÇÕES?: TEORIA DOS LÍQUIDOS DE FERMI:

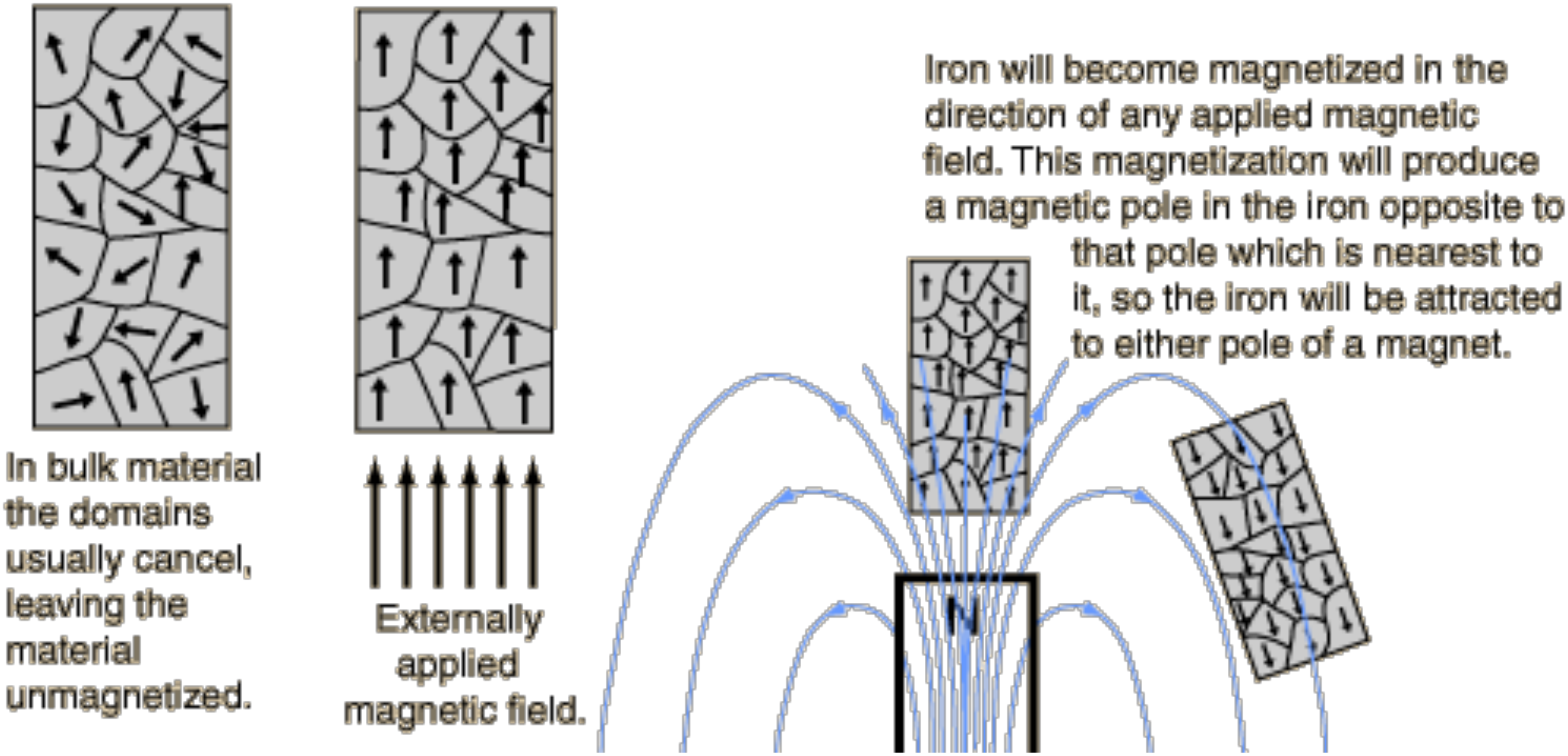
(a) EXCITAÇÕES ELEMENTARES ESTÃO NUMA CORRESPONDÊNCIA UM PARA UM COM AS DO SISTEMA LIVRE.

b) AS MASSAS EFETIVAS DOS QUASE-ELÉTRONS (BURACOS)

$m^* > m$

c) HÁ INTERAÇÕES EFETIVAS ENTRE AS QUASE-PARTÍCULAS QUE AFETAM AS QUANTIDADES FÍSICAS

Defeitos:
Ferromagnetismo e domínios



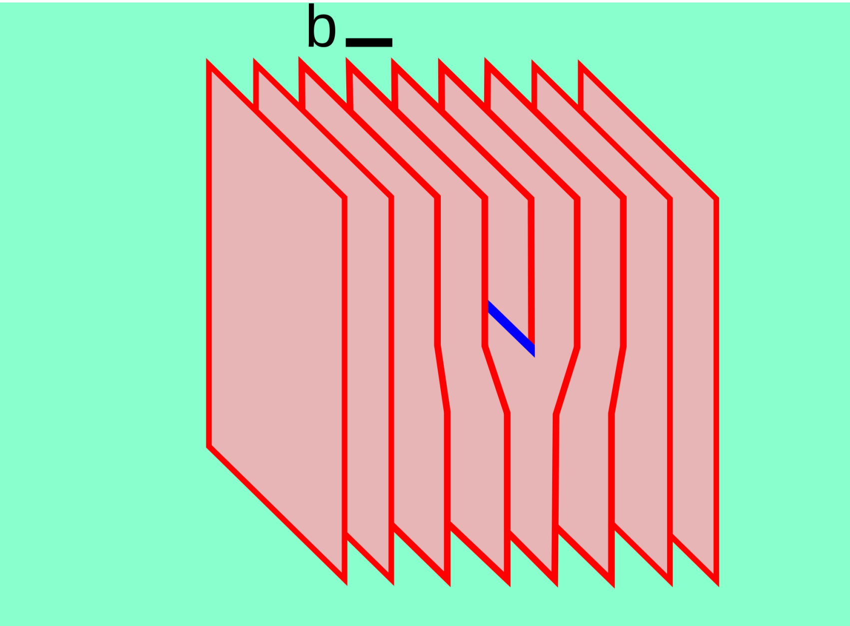
In bulk material the domains usually cancel, leaving the material unmagnetized.

Externally applied magnetic field.

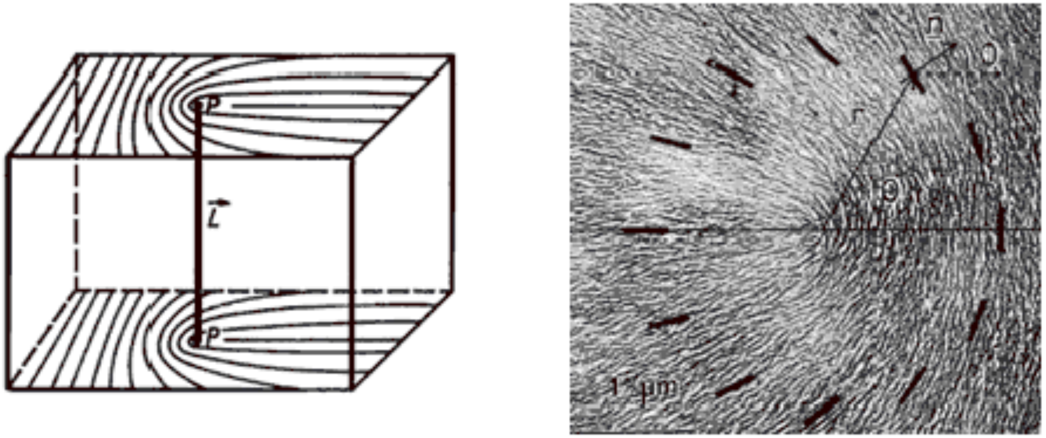
Iron will become magnetized in the direction of any applied magnetic field. This magnetization will produce a magnetic pole in the iron opposite to that pole which is nearest to it, so the iron will be attracted to either pole of a magnet.

Defeitos

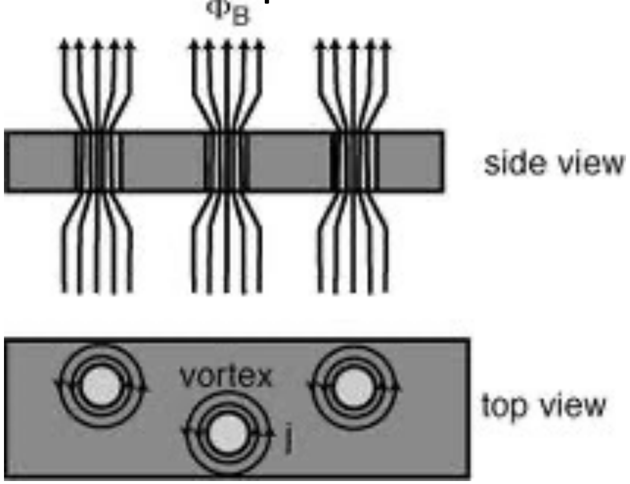
Discordância



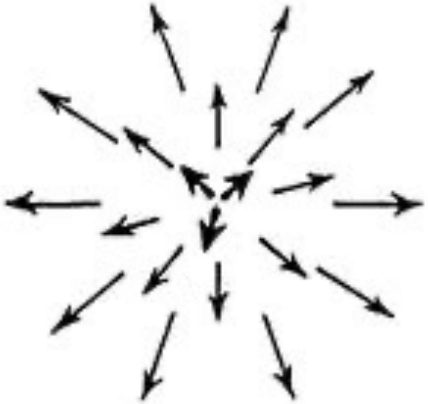
Disclinação em cristal líquido



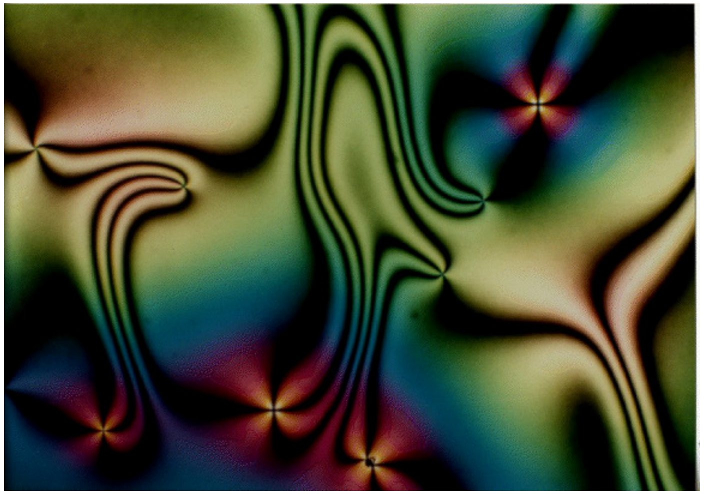
Vórtice supercondutor



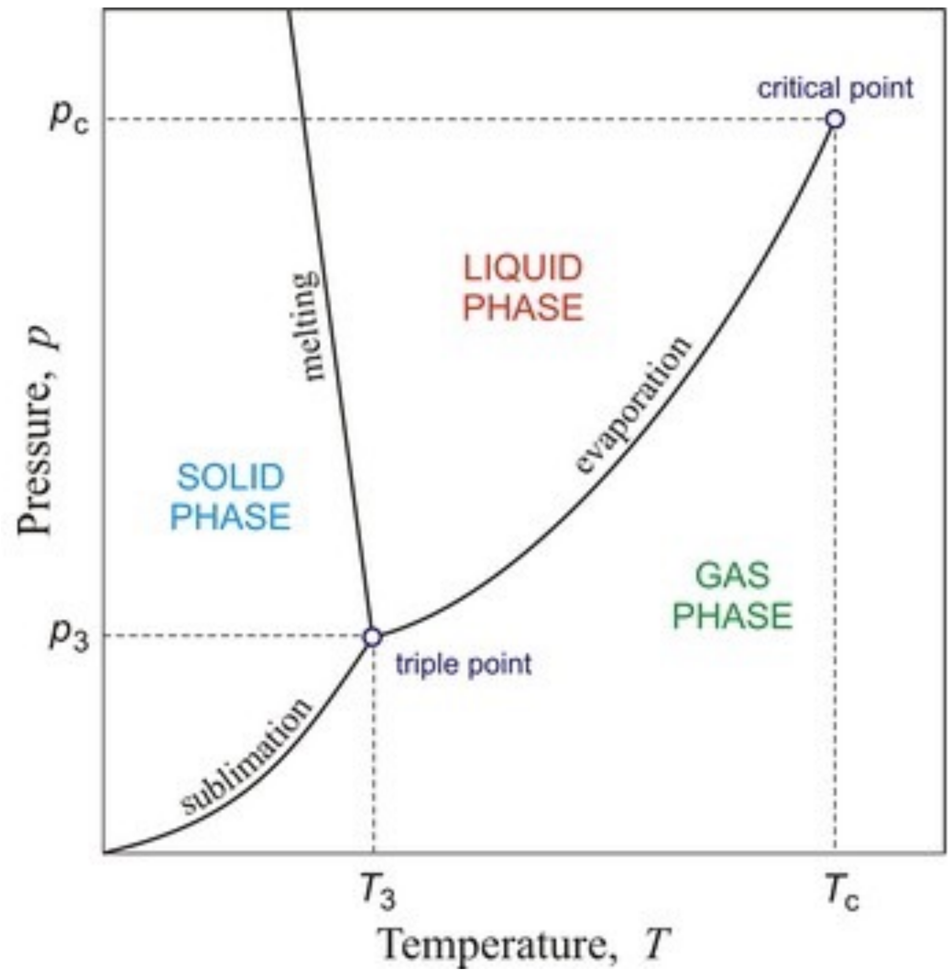
Porco-espinho

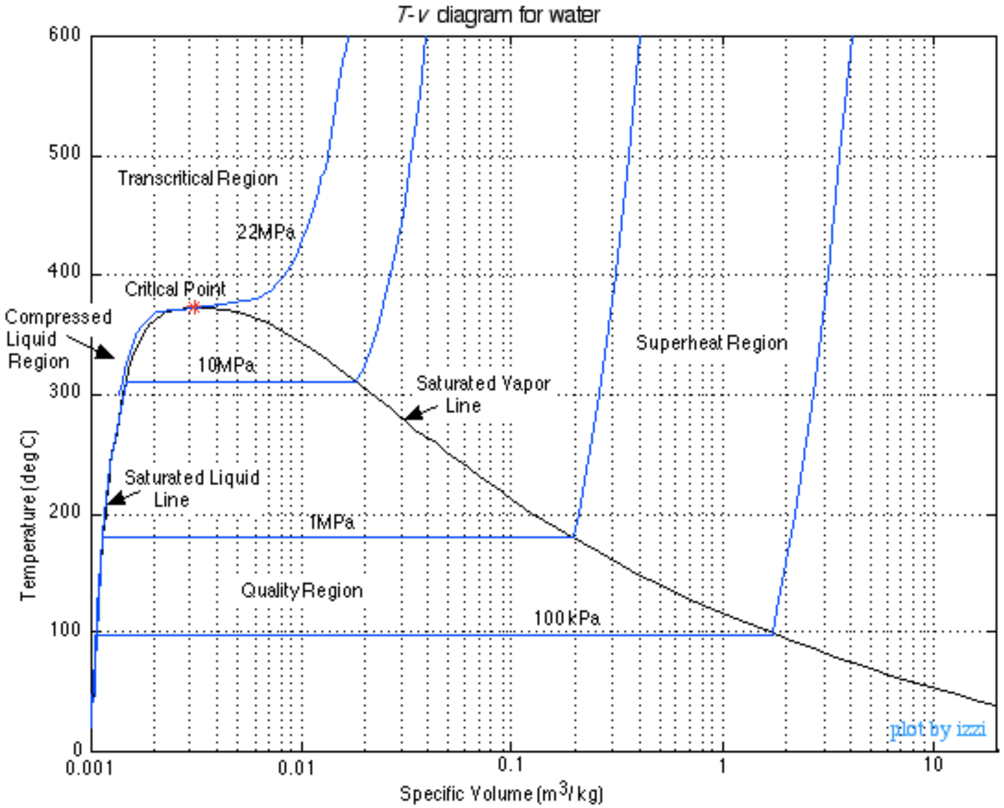


Boojum em um nemático

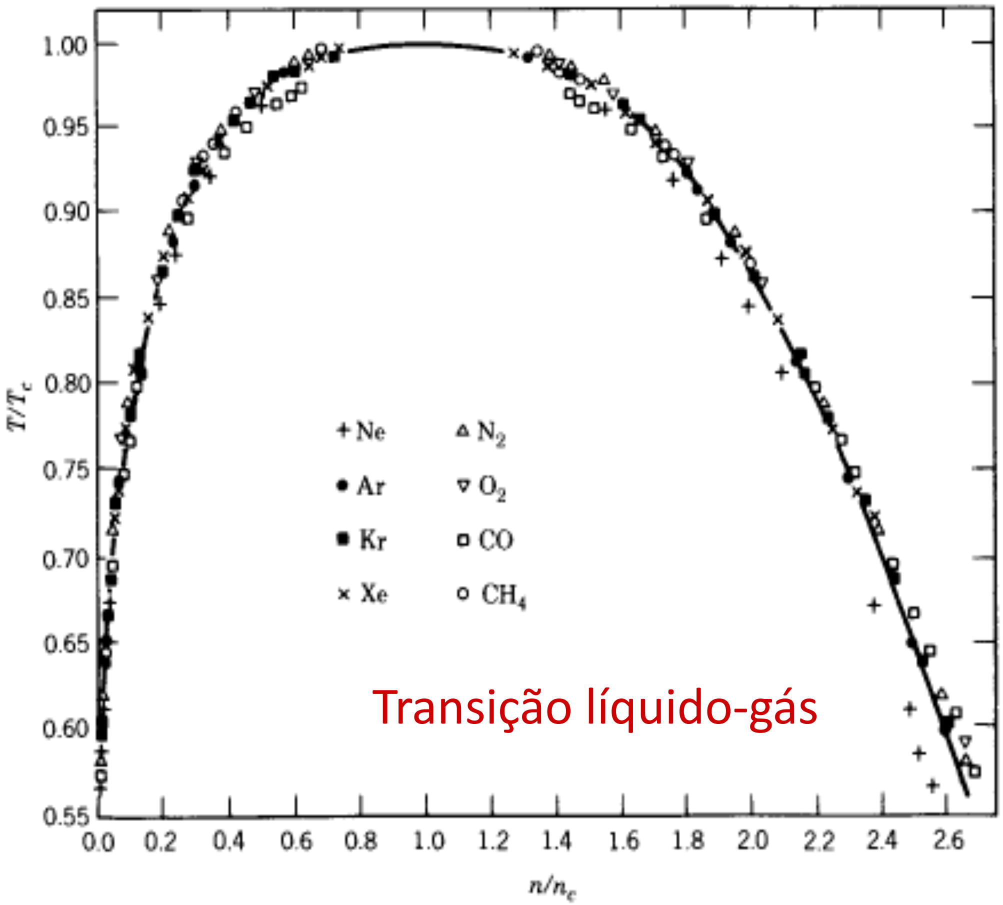


Universalidade





Universalidade



Transição líquido-gás

Fig. 16.2 Reduced temperature vs. reduced density in the gas-liquid coexistence region, for eight different substances.

Expoentes críticos

$$M(T) = \mathrm{Tr}\left\{\frac{e^{-\beta H}}{Z} S(\mathbf{r})\right\} \text{ ferromagneto}$$

$$\rho(T) = \mathrm{Tr}\left\{\frac{e^{-\beta H}}{Z} \rho(\mathbf{r})\right\} \text{ líquido} - \text{gás}$$

$$C_V(T) \sim \frac{1}{|T - T_c|^{\boxed{\alpha}}}$$

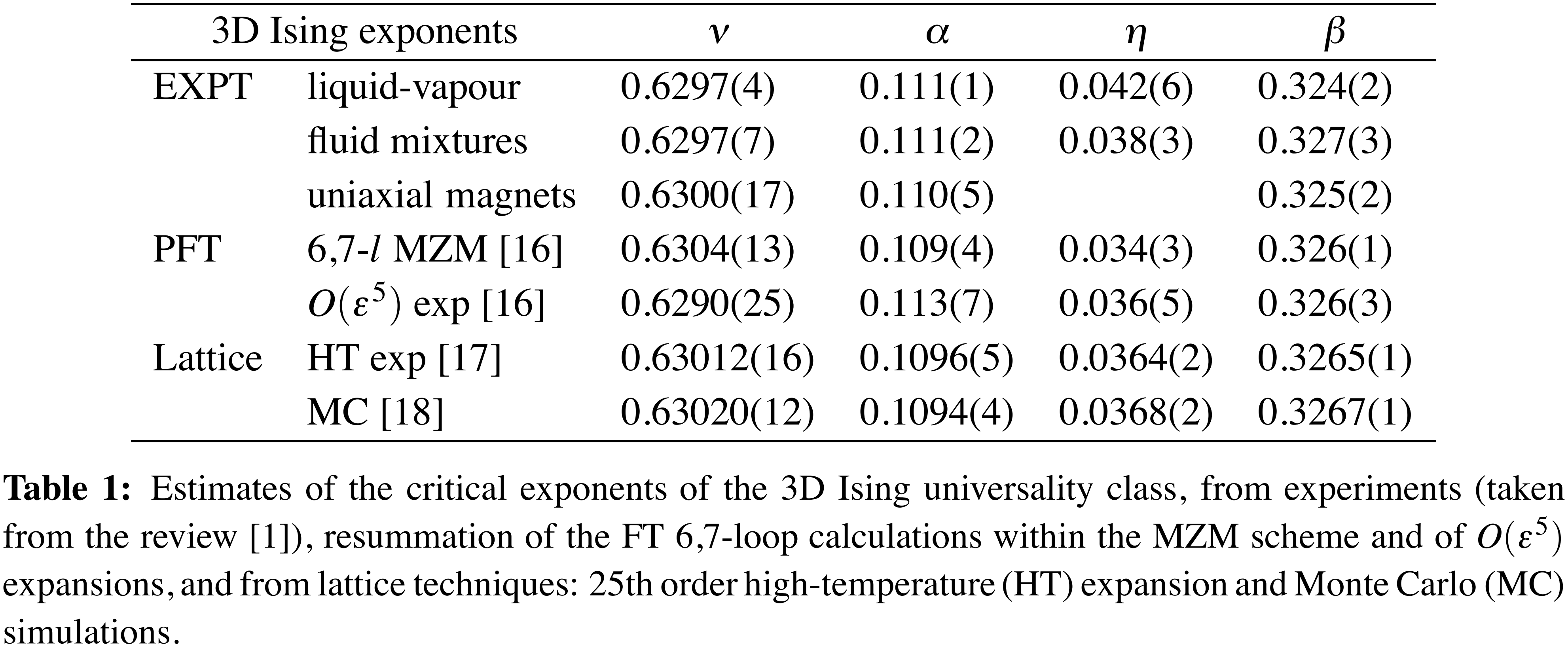
$$O(\mathbf{r}) = \begin{cases} S(\mathbf{r}) - M(T) & \text{ferromagneto} \\ \rho(\mathbf{r}) - \rho(T) & \text{líquido} - \text{gás} \end{cases}$$

$$T < T_c : \begin{cases} M(T) \sim (T_c - T)^{\boxed{\beta}} \\ \rho_l(T) - \rho_g(T) \sim (T_c - T)^{\boxed{\beta}} \end{cases}$$

$$G(\mathbf{r}) = \mathrm{Tr}\left\{\frac{e^{-\beta H}}{Z} O(\mathbf{r}) O(0)\right\} \sim \begin{cases} e^{-r/\xi(T)}/r^{(d-1)/2} & T < T_c \text{ ou } T > T_c \\ 1/r^{d-2\boxed{+\eta}} & T = T_c \end{cases}$$

$$\xi(T) \sim \frac{1}{|T - T_c|^{\boxed{\nu}}}$$

Expoentes críticos



3D Ising exponents		ν	α	η	β
EXPT	liquid-vapour	0.6297(4)	0.111(1)	0.042(6)	0.324(2)
	fluid mixtures	0.6297(7)	0.111(2)	0.038(3)	0.327(3)
	uniaxial magnets	0.6300(17)	0.110(5)		0.325(2)
PFT	6,7-l MZM [16]	0.6304(13)	0.109(4)	0.034(3)	0.326(1)
	$O(\varepsilon^5)$ exp [16]	0.6290(25)	0.113(7)	0.036(5)	0.326(3)
Lattice	HT exp [17]	0.63012(16)	0.1096(5)	0.0364(2)	0.3265(1)
	MC [18]	0.63020(12)	0.1094(4)	0.0368(2)	0.3267(1)

Table 1: Estimates of the critical exponents of the 3D Ising universality class, from experiments (taken from the review [1]), resummation of the FT 6,7-loop calculations within the MZM scheme and of $O(\varepsilon^5)$ expansions, and from lattice techniques: 25th order high-temperature (HT) expansion and Monte Carlo (MC) simulations.

E. Vicari, *Critical phenomena and renormalization-group flow of multi-parameter Φ^4 field theories*, PoSLAT2007, 023 (2007)