

FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

2º Semestre de 2023

24/08/2023

Aula 7

Modelo de Hubbard

$$H_{\text{Hubbard}} = \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + U \sum_{i\sigma} n_{i\uparrow} n_{i\downarrow}$$

EM SEMI-PREENCHIMENTO: $\frac{N_e}{N_s} = 1 = \nu$

EM $D \gg 1$:

$U \ll t \rightarrow$ BANDA SEMI-PREENCHIDA
METAL

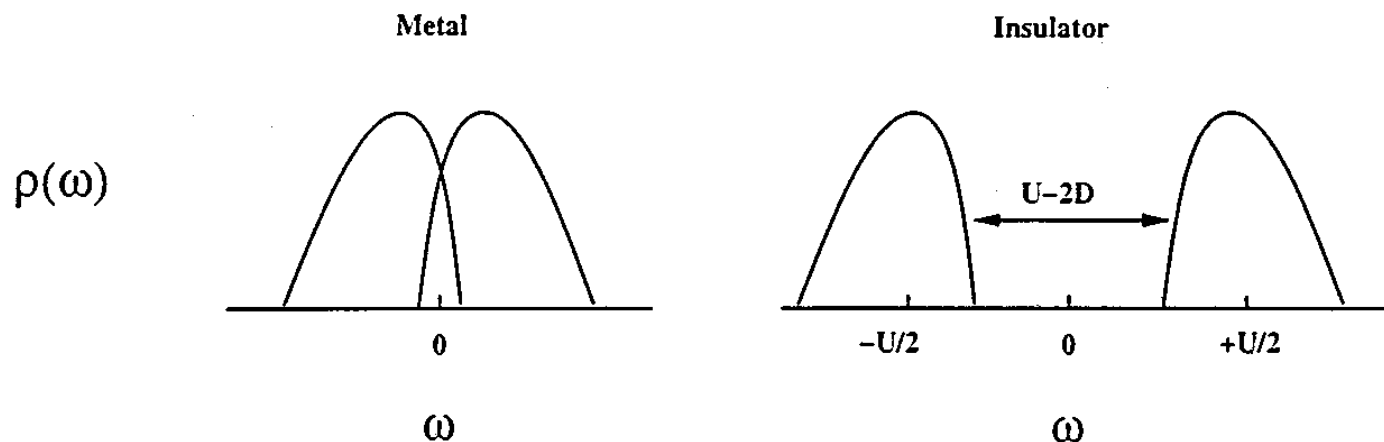
$U \gg t \rightarrow$ UM ELÉTRON LOCALIZADO
POR SÍTIO. PAGAR ENERGIA
 U PARA MOVER CADA ELÉTRON
ISOLANTE DE MOTT

TRANSIÇÃO METAL-ISOLANTE

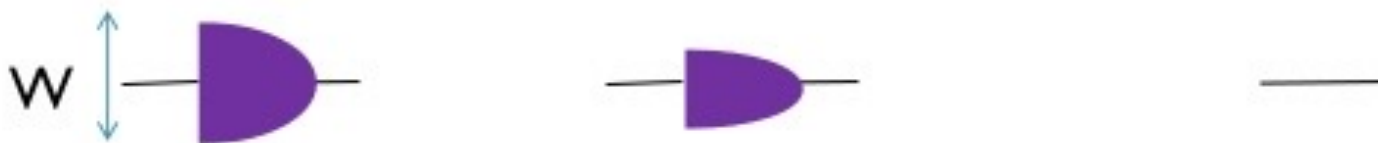
PARA $U = U_c$

Primeiras descrições teóricas

- A descrição de Hubbard III: do isolante para o metal; duas bandas (de Hubbard) separadas que se tocam na transição ([J. Hubbard, Proc. R. Soc. \(London\) A 281, 401 \(1964\)](#))



- A descrição de Brinkman e Rice: do metal para o isolante; desaparecimento das quasi-partículas, $m^* \rightarrow \infty$; não há bandas de Hubbard ([W. F. Brinkman and T. M. Rice, Phys. Rev. B 2, 4302 \(1970\)](#))

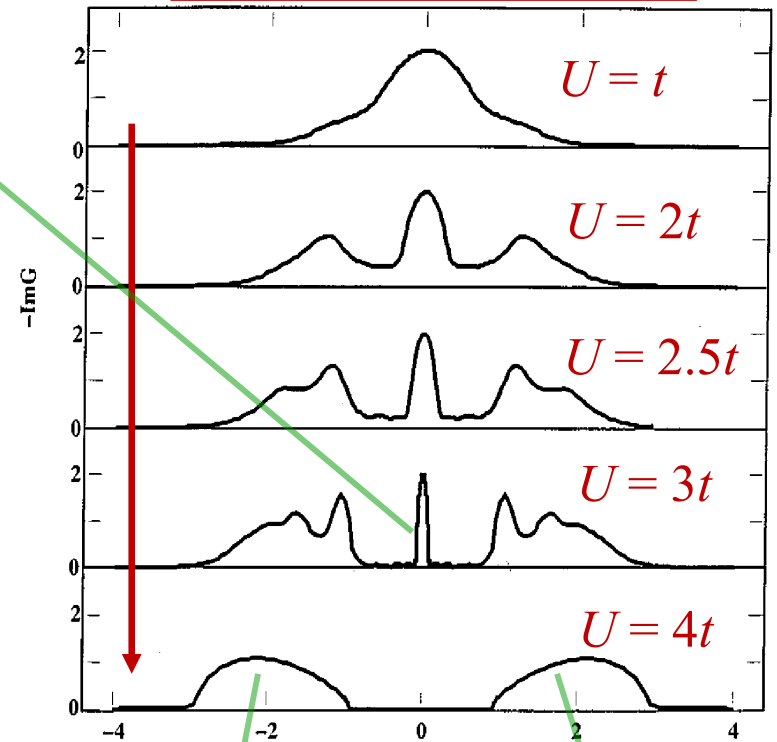


Teoria dinâmica de campo médio (Dynamical mean field theory)

Pico de quasi-partículas (Brinkman-Rice)

Unificação de Brinkman-Rice + Hubbard III

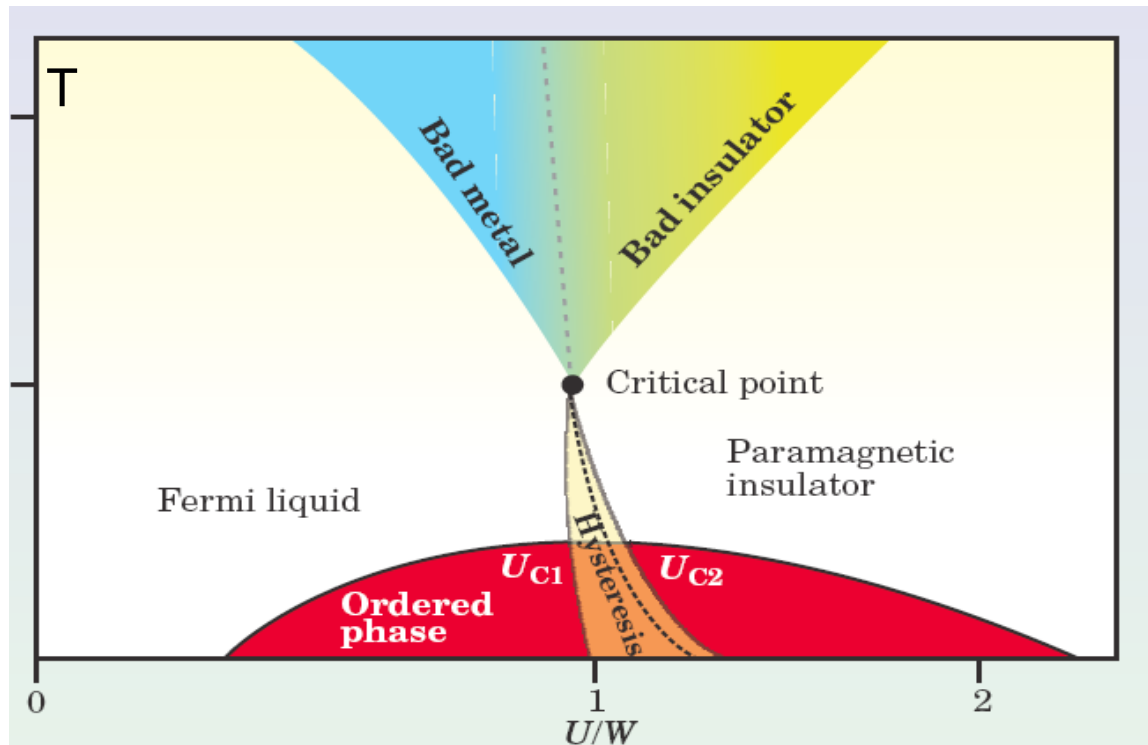
Density of states



X.Y.Zhang, M. Rozenberg G. Kotliar (PRL 1993)

Bandas de Hubbard (Hubbard III)

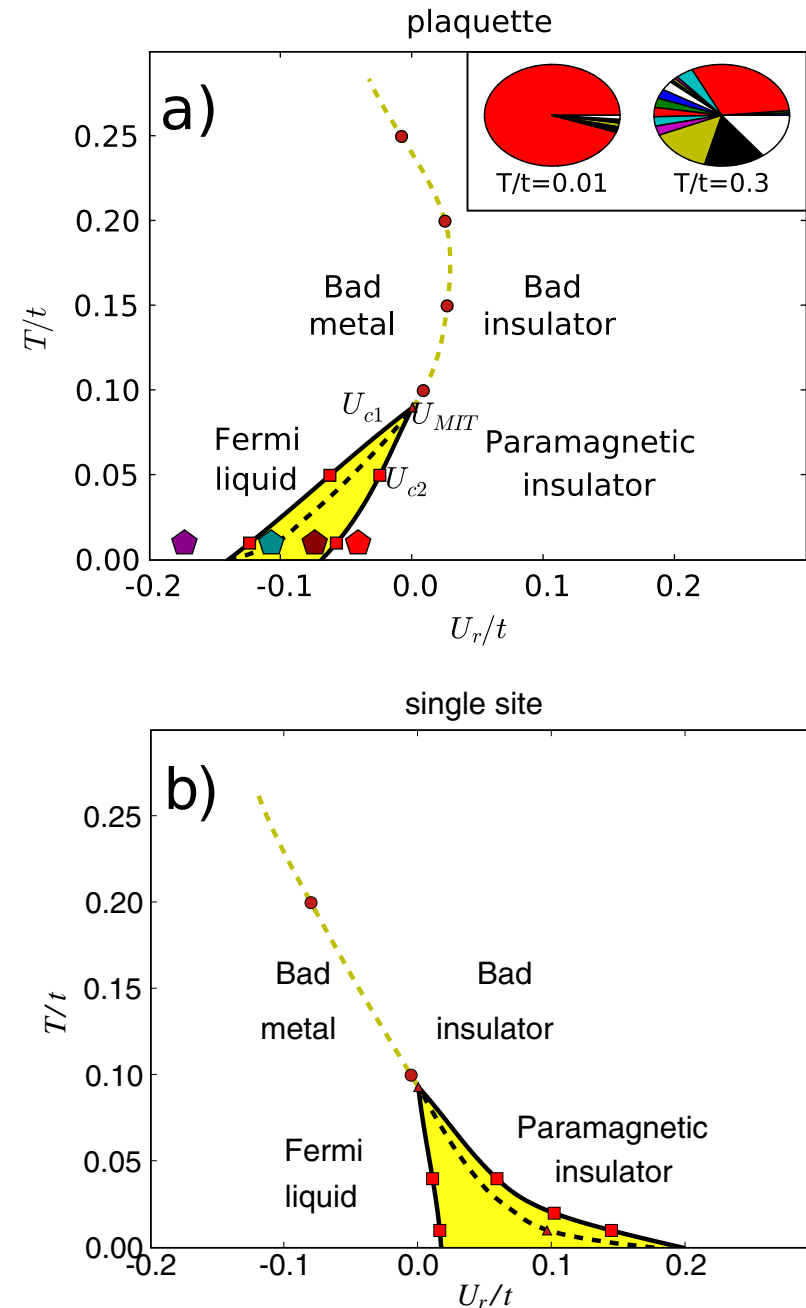
Diagrama de fases (DMFT)



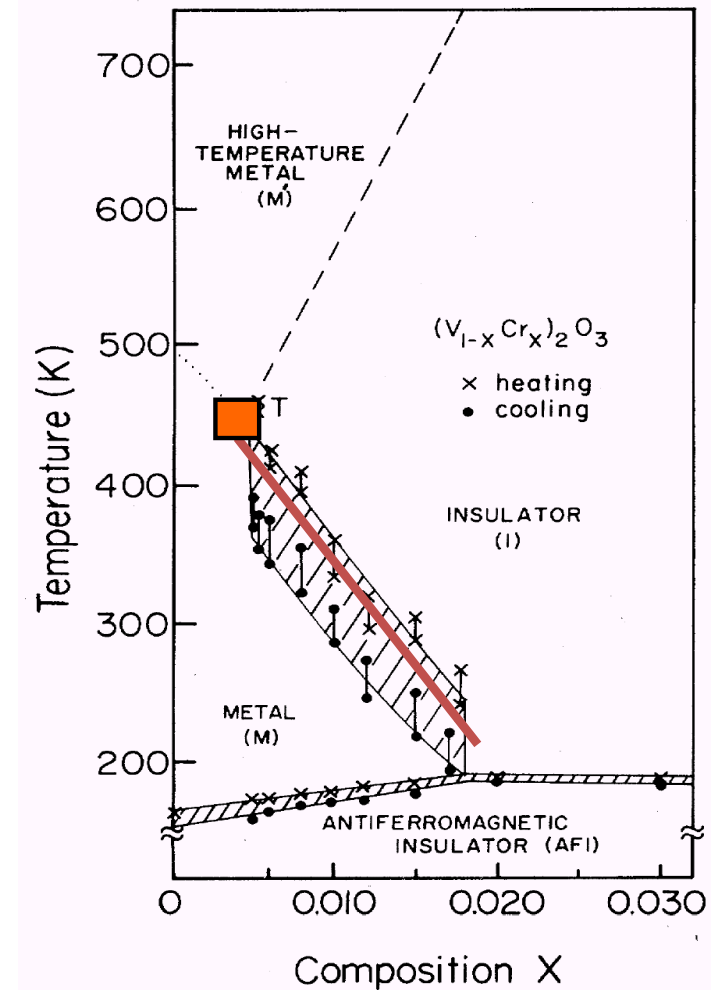
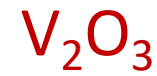
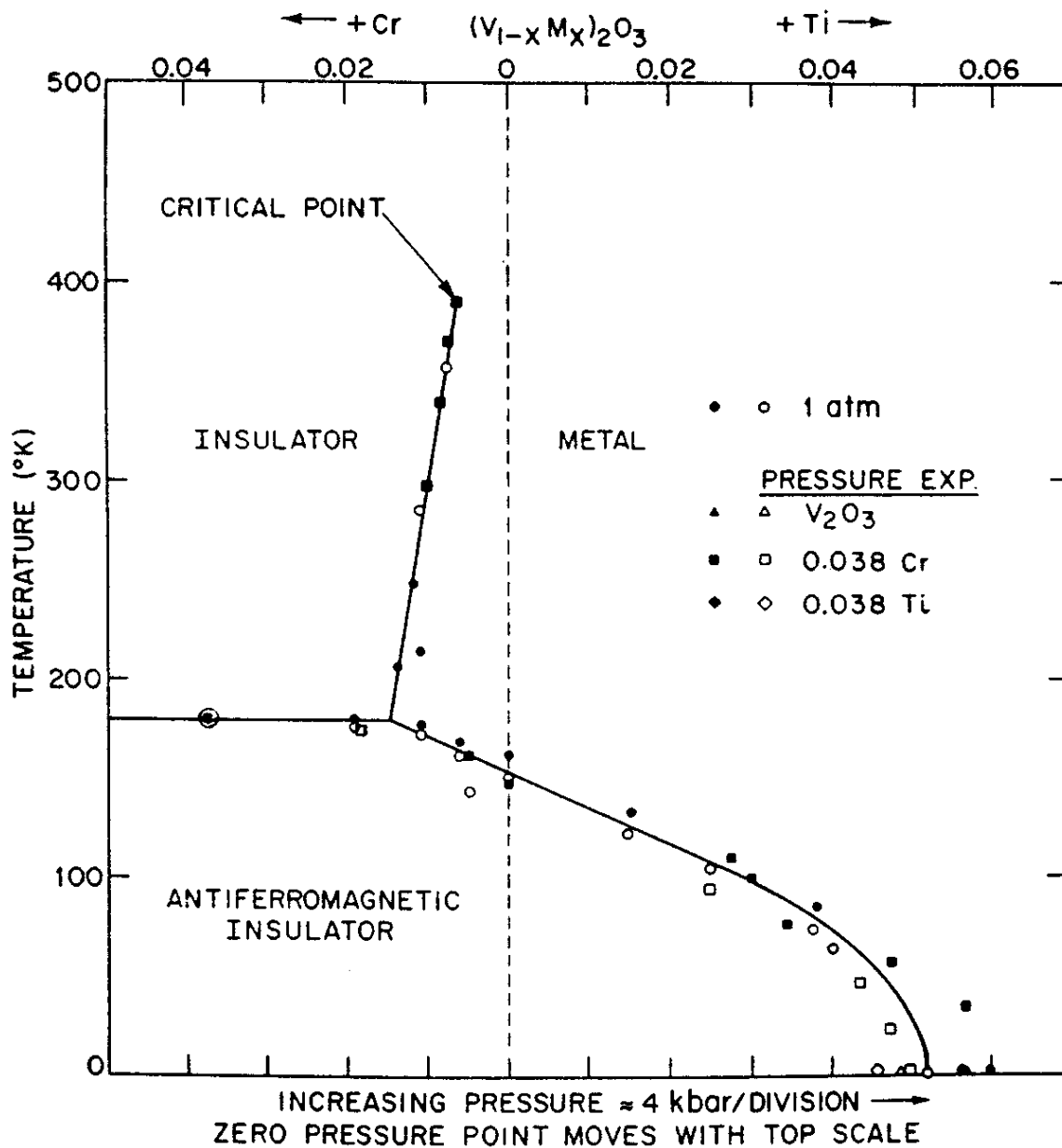
Kotliar, Vollhardt, Phys. Today (2004)

Além da DMFT: cluster DMFT

H. Park, K. Haule, and G. Kotliar
Phys. Rev. Lett. **101**, 186403 (2008).



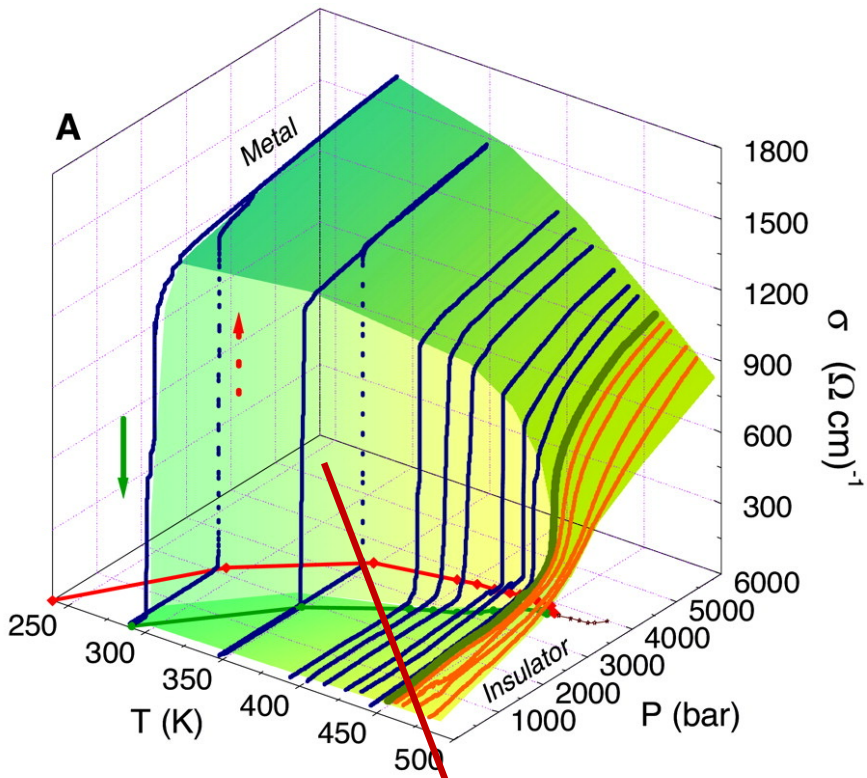
McWhan, D. B., A. Menth, J. P. Remeika, W. F. Brinkman, and T. M. Rice, 1973, Phys. Rev. B 7, 1920.



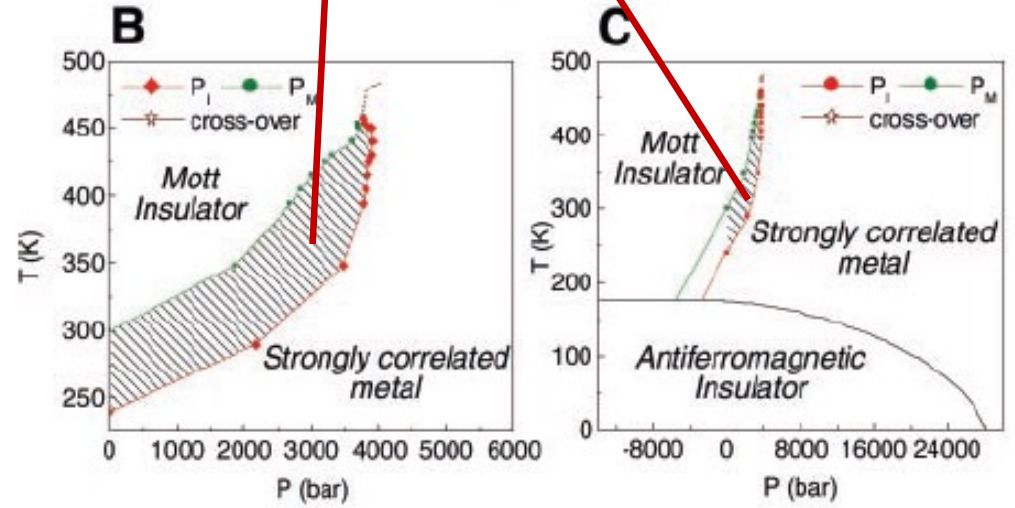
Kuwamoto, PRB '80

- Pressão aumenta t , diminui U/t , favorece o comportamento metálico.
- Pressão química: elemento de raio iônico maior/menor aumenta o parâmetro de rede e age como pressão negativa/positiva.

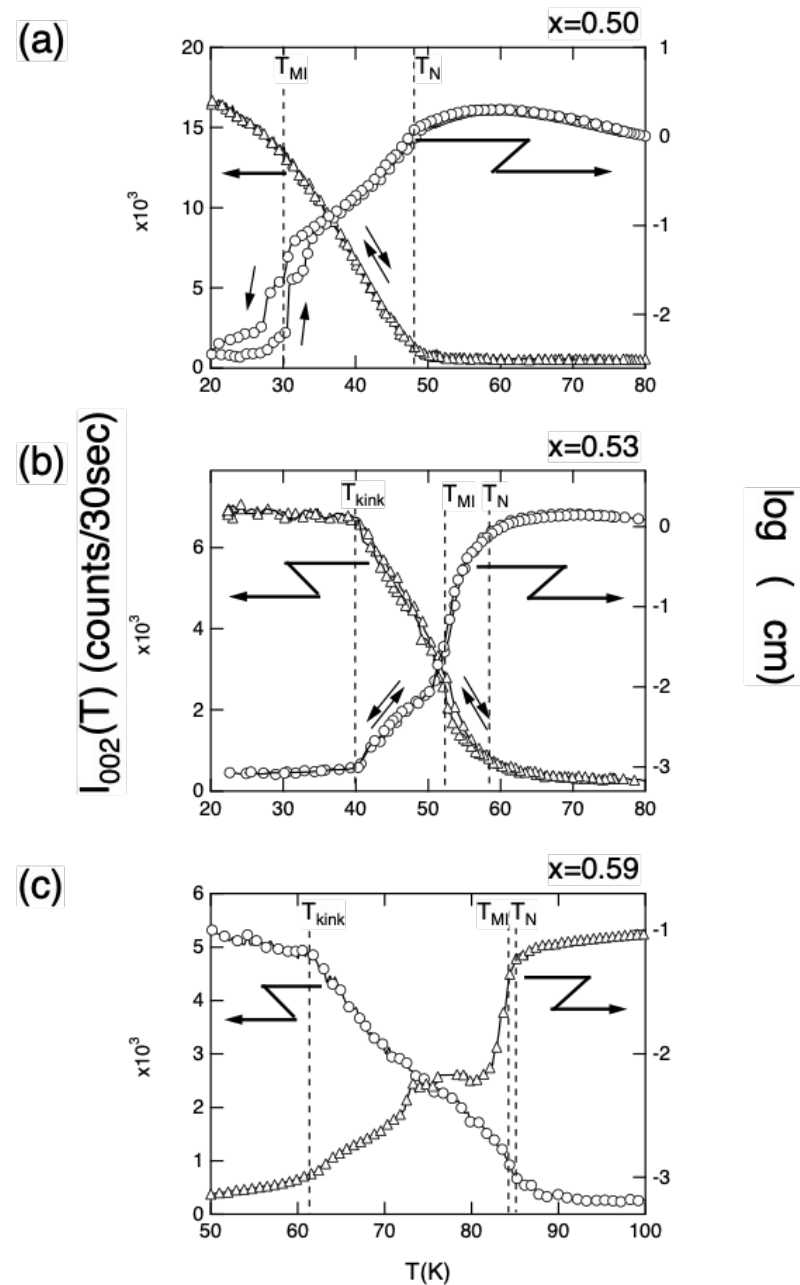
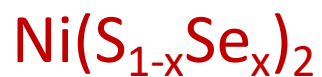
Experimentos em $(V_{0.989}Cr_{0.011})_2O_3$ sob pressão (P. Limelette *et al.*, Science **302**, 89 (2003)).



Coexistência metal-isolante

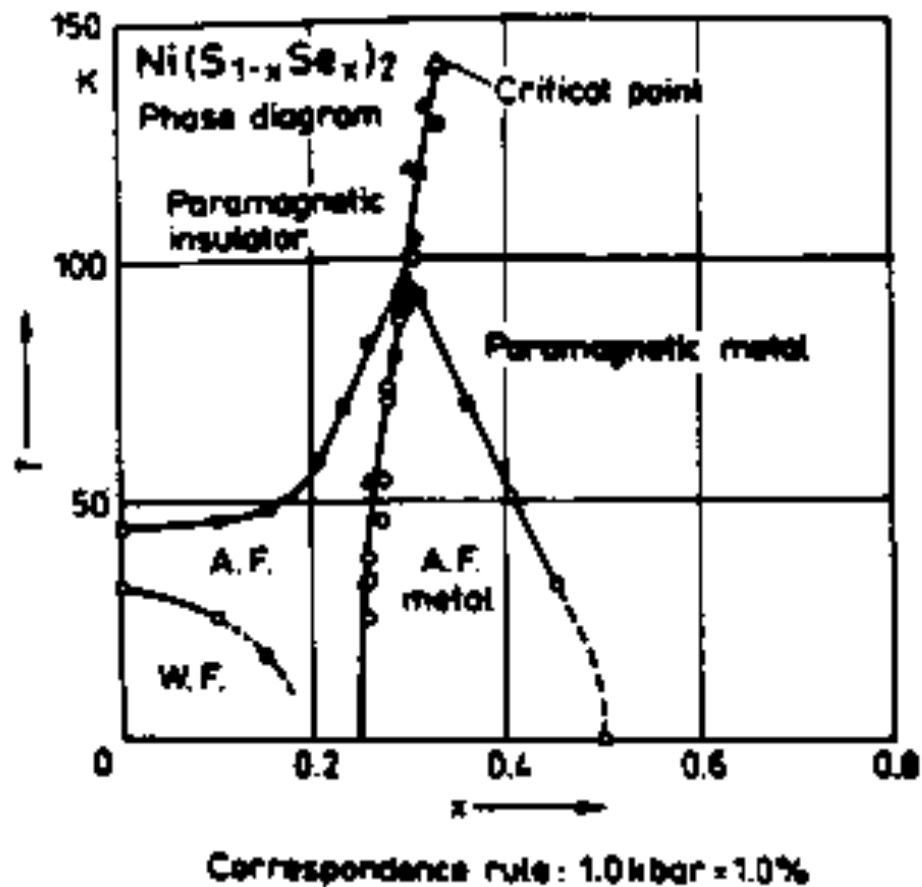
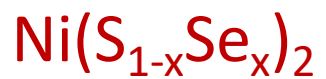


- Histerese: transição de primeira ordem
- Note como a linha de transições termina num ponto crítico
- Como a transição líquido-gás!



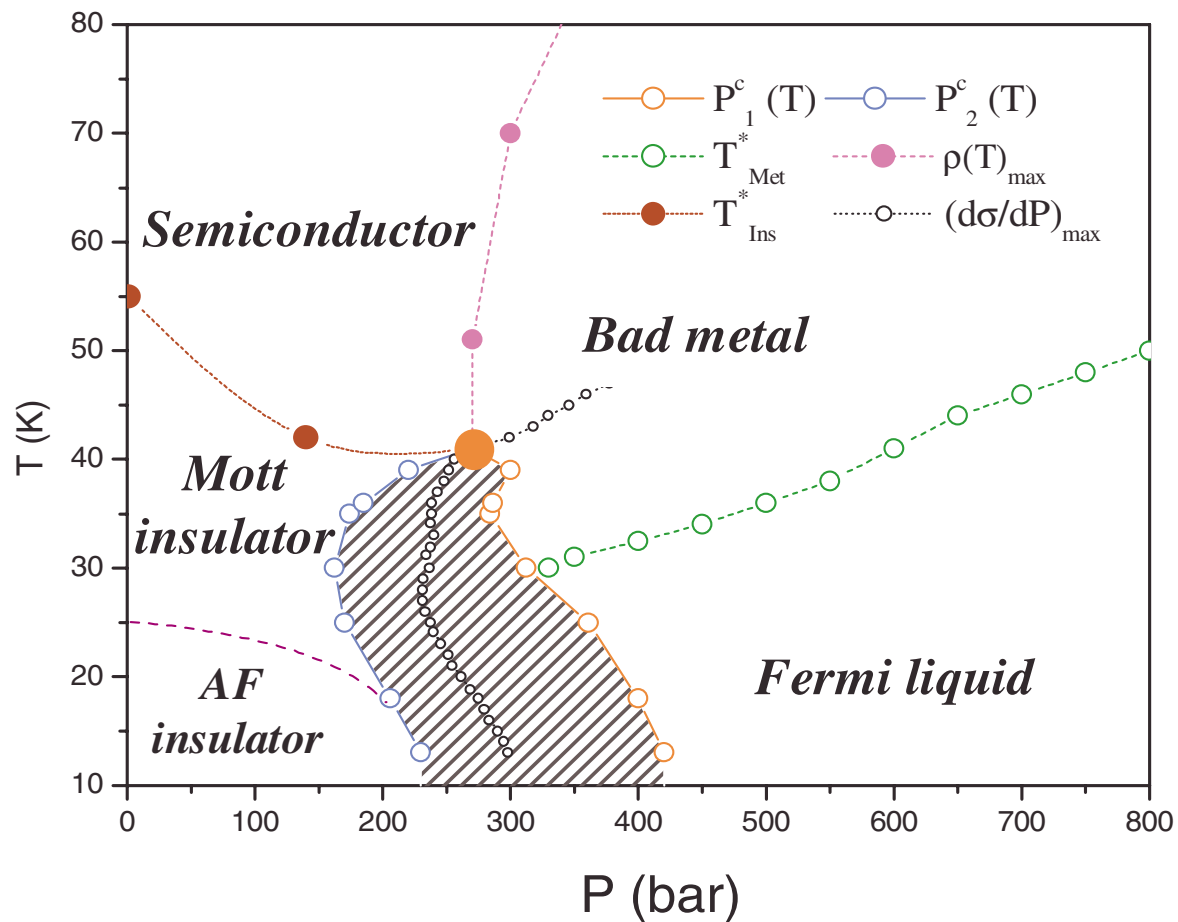
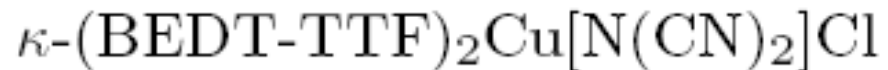
M. Matsuura *et al.*, J. Phys. Soc. Jpn
69, 1503 (2000)

Fig. 5. Temperature dependences of the electrical resistivity and the peak intensity of (002) antiferromagnetic Bragg reflection, $I_{002}(T)$ measured simultaneously for (a) $x = 0.50$ and (b) $x = 0.53$, and separately for (c) $x = 0.59$. Circles and triangles indicate electrical resistivity and $I_{002}(T)$, respectively.



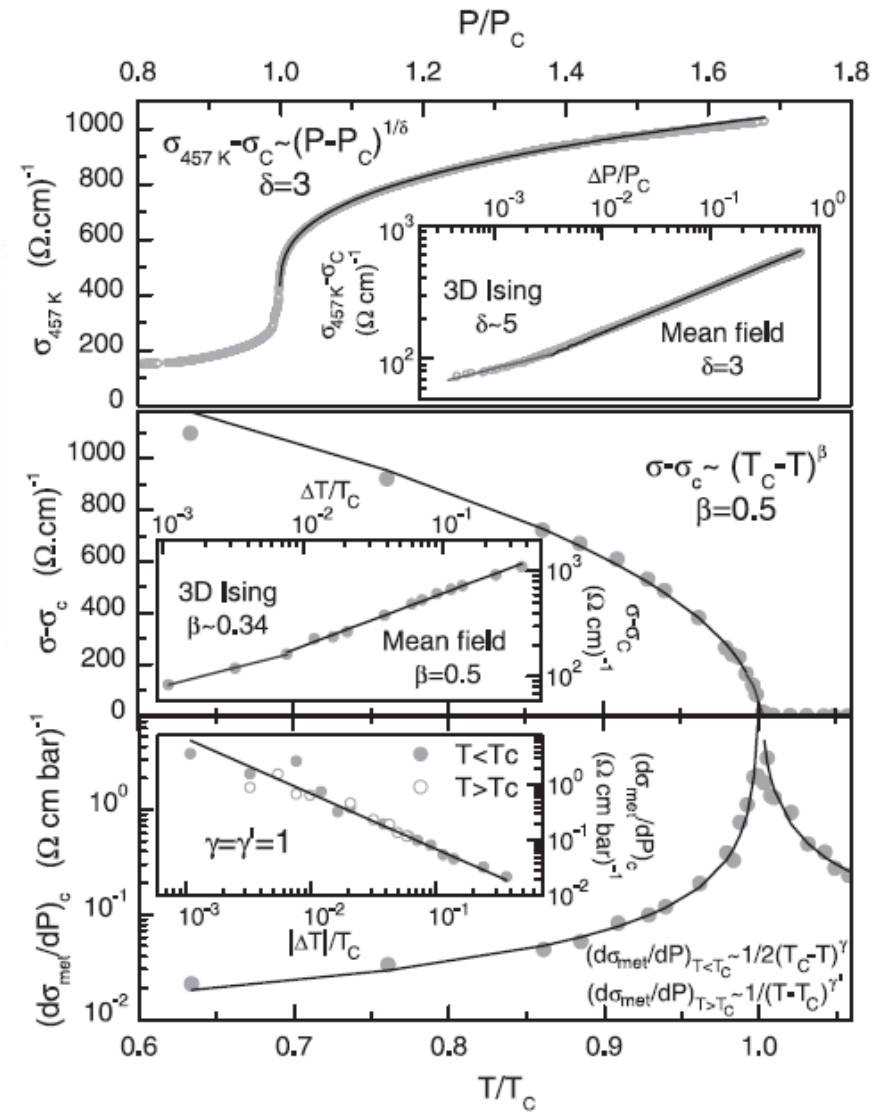
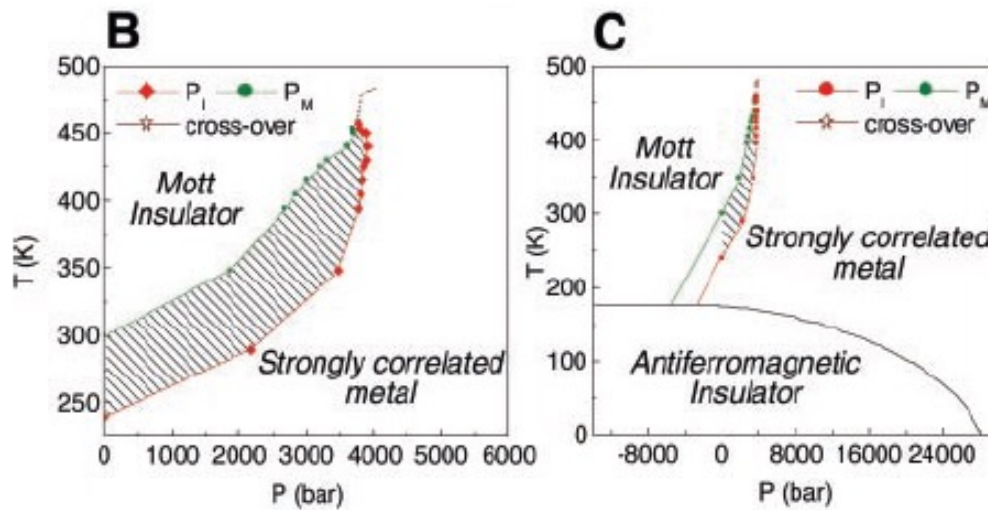
Czjzek *et al.*, JMMM 3, 58 (1976)

Condutores orgânicos fortemente bi-dimensionais



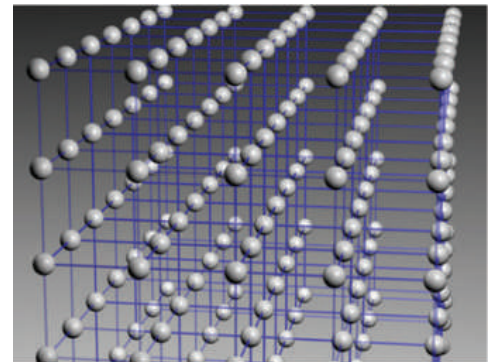
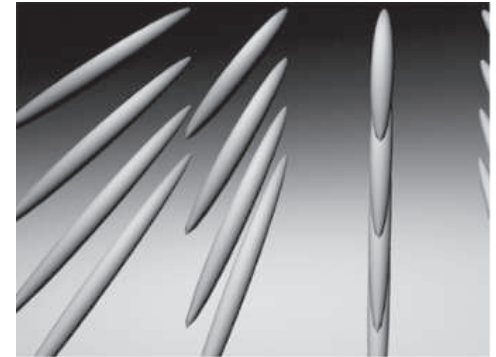
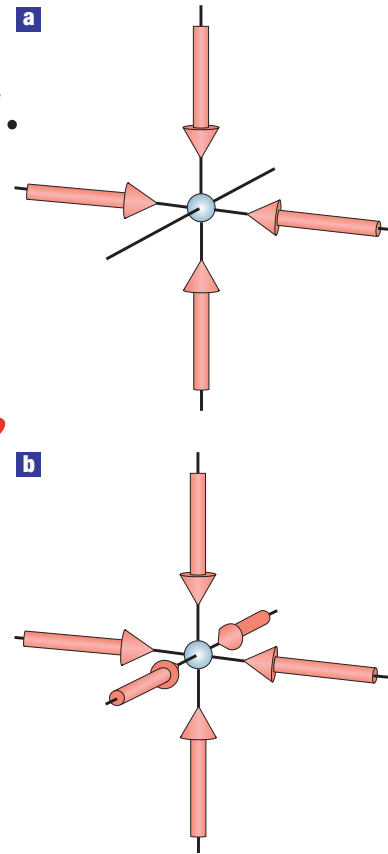
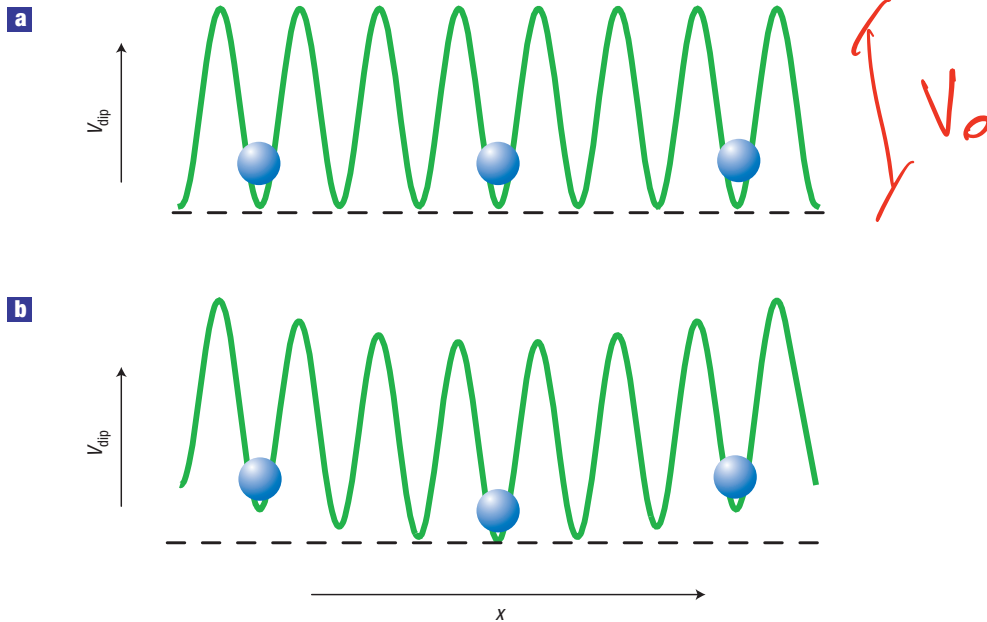
Transição de Mott: o ponto crítico

Comportamento crítico idêntico ao da **transição líquido gás** (classe de universalidade de Ising).



O modelo de Hubbard para átomos frios: redes ópticas

$$V_{\text{dip}}(\mathbf{r}) = -\mathbf{d} \cdot \mathbf{E}(\mathbf{r}) \propto \alpha(\omega_L) |\mathbf{E}(\mathbf{r})|^2.$$



Immanuel Bloch, Nature Phys. 1, 23 (2005)

Modelo de Bose-Hubbard

BÓSONS DE SPIN $S=0$; MODELO BOSE-HUBBARD

$$H = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i b_i^\dagger b_i^\dagger b_i b_i$$

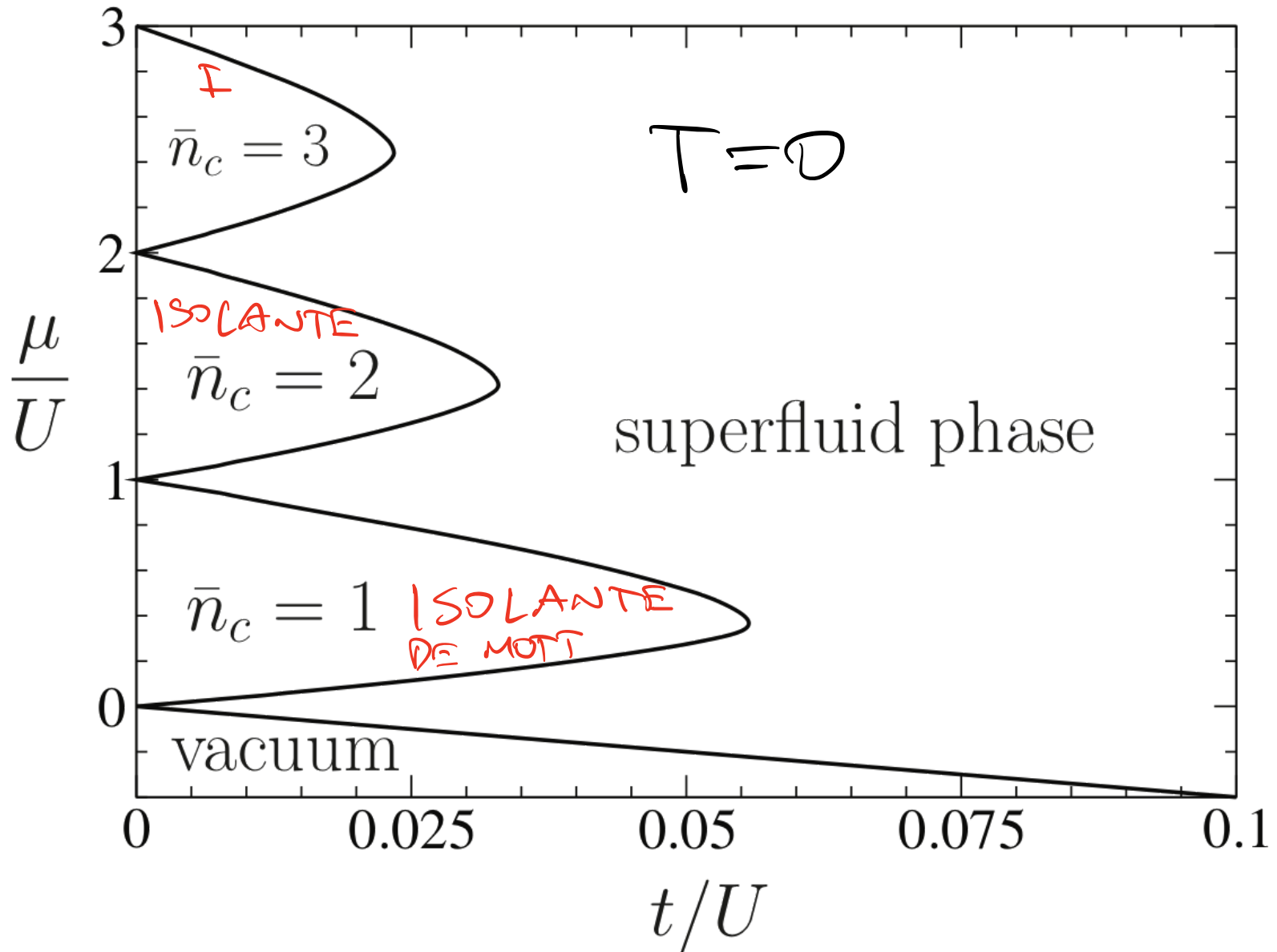
$$b_i^\dagger b_i^\dagger b_i b_i = b_i^\dagger [b_i b_i^\dagger - 1] b_i = n_i n_i - n_i = n_i(n_i - 1)$$

$$[b_i, b_i^\dagger] = b_i b_i^\dagger - b_i^\dagger b_i = 1$$

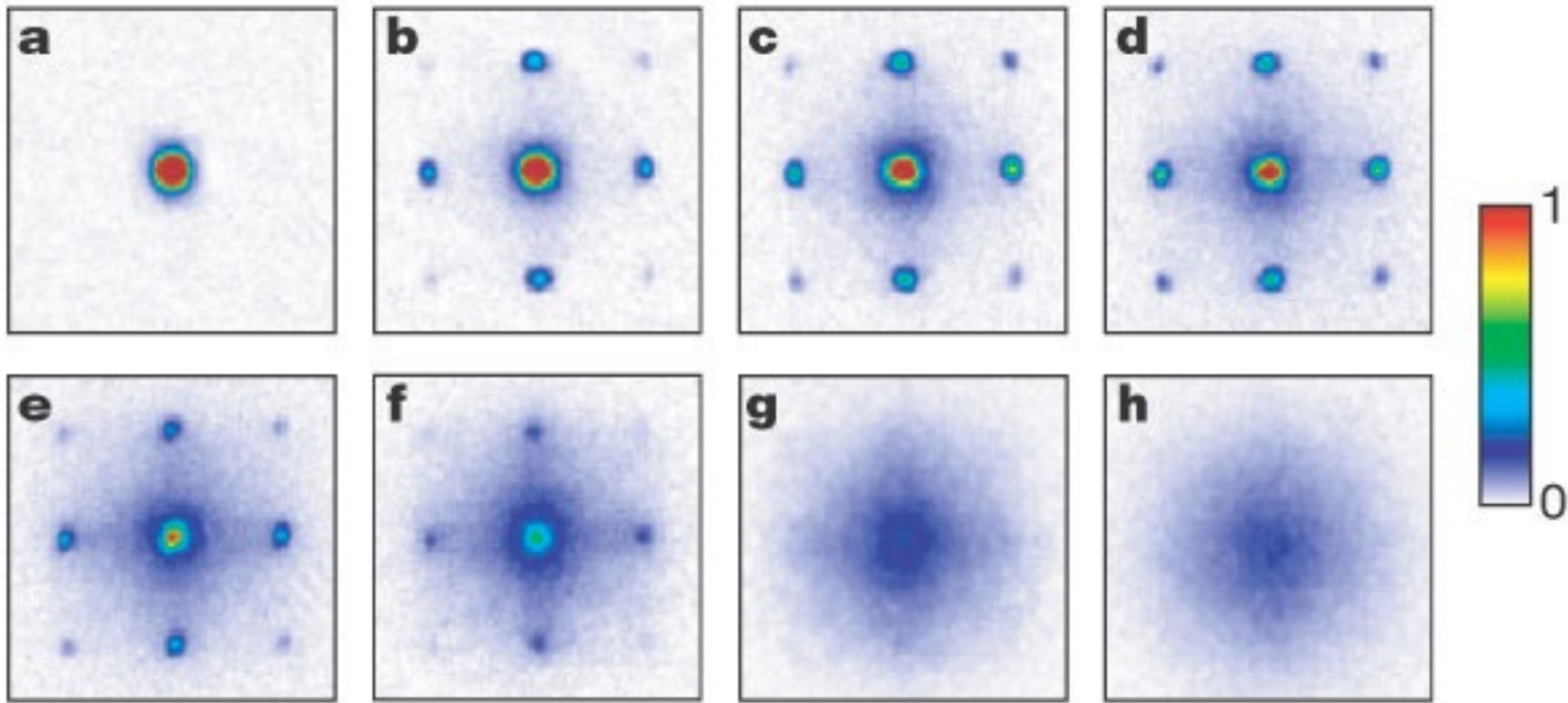
$$H = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + h.c.) + \frac{U}{2} \sum_i n_i(n_i - 1)$$

$U \ll t$: SUPERFLUIDO } EM PREENCHIMENTO
 $U \gg t$: ISOLANTE } INTEIRO ($n=1, 2, 3, \dots$)

Diagrama de fases



Transição superfluido-isolante de Mott: ^{87}Rb



Markus Greiner *et al.*, Nature **415**, 39 (2002)

These were obtained after suddenly releasing the atoms from an optical lattice potential with different potential depths V_0 after a time of flight of 15 ms. Values of V_0 were: a, 0 Er; b, 3 Er; c, 7 Er; d, 10 Er; e, 13 Er; f, 14 Er; g, 16 Er; and h, 20 Er.

Isolante de Mott

O modelo de Heisenberg e superexchange

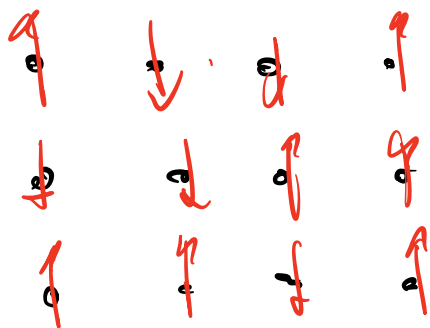
EM SEMI-PREENCHIMENTO: $\mu = 1$ E BEM DENTRO

DA FASE ISOLANTE: $U \gg t$

TRATAR O SISTEMA POR T. DE PERT. EM $\frac{t}{U}$

$$H_0 = U \sum_i n_{i\uparrow} n_{i\downarrow} \quad H_1 = -t \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.)$$

EM ORDEM ZERO: UM ELÉTRON POR SÍTIO COM SPIN ARBITRÁRIO:



$$\Rightarrow |\sigma_1 \sigma_2 \dots \sigma_{N_s}\rangle = c_{1\sigma_1}^\dagger c_{2\sigma_2}^\dagger \dots c_{N_s \sigma_{N_s}}^\dagger |0\rangle$$

2^{N_s} ESTADOS POSSÍVEIS

$$E^{(0)} = 0$$

EM 1ª ORDEM: $\langle \sigma_1 \sigma_2 \dots \sigma_{N_s} | H_2 | \sigma_2' \sigma_2' \dots \sigma_{N_s}' \rangle = 0$
 $\hookrightarrow \langle \alpha | H_1 | \beta \rangle$

CADA TERMO DE H_1 TRANSFERE UM ELÉTRON PRO

SÍTIO VIZINHO, CONSERVANDO SPIN: CRIA UMA

VACÂNCIA NUM SÍTIO E UMA DUPLA OCUPAÇÃO NO VIZINHO.

PRECISO IR PARA 2ª ORDEM: ESTADO GÊNÉRICO $\rightarrow |\alpha\rangle$

$$H_{\alpha\beta}^{(2)} = \sum_{m \neq 0} \frac{\langle \alpha | H_1 | m \rangle \langle m | H_2 | \beta \rangle}{E_0 - E_m}$$

CADA $|m\rangle$ NA SOMA TEM UMA VACÂNCIA E UMA DUPLA OCUPAÇÃO NUM VIZINHO E OS OUTROS ESTADOS OCUPADOS POR UM ELÉTRON APENAS.

$$E_N = U \quad E_0 = 0$$

DA SOMA SOBRE m APENAS SOBRA M OS ESTADOS
 COM 1 V. E 1 D.O. $\rightarrow |m\rangle$, POIS TODOS OS OUTROS
 ESTADOS DÃO $\langle m | H_1 | \beta \rangle \Rightarrow$

RESTRINGINDO A SOMA A ESTES ESTADOS,
 PODEMOS TIRAR $\frac{1}{E_0 - E_m} = -\frac{1}{U}$ PARA FORA DA

SOMA:

$$H_{\alpha\beta}^{(2)} = \left(-\frac{1}{U}\right) \sum_{m1} \langle \alpha | H_1 | m' \rangle \langle m' | H_2 | \beta \rangle$$

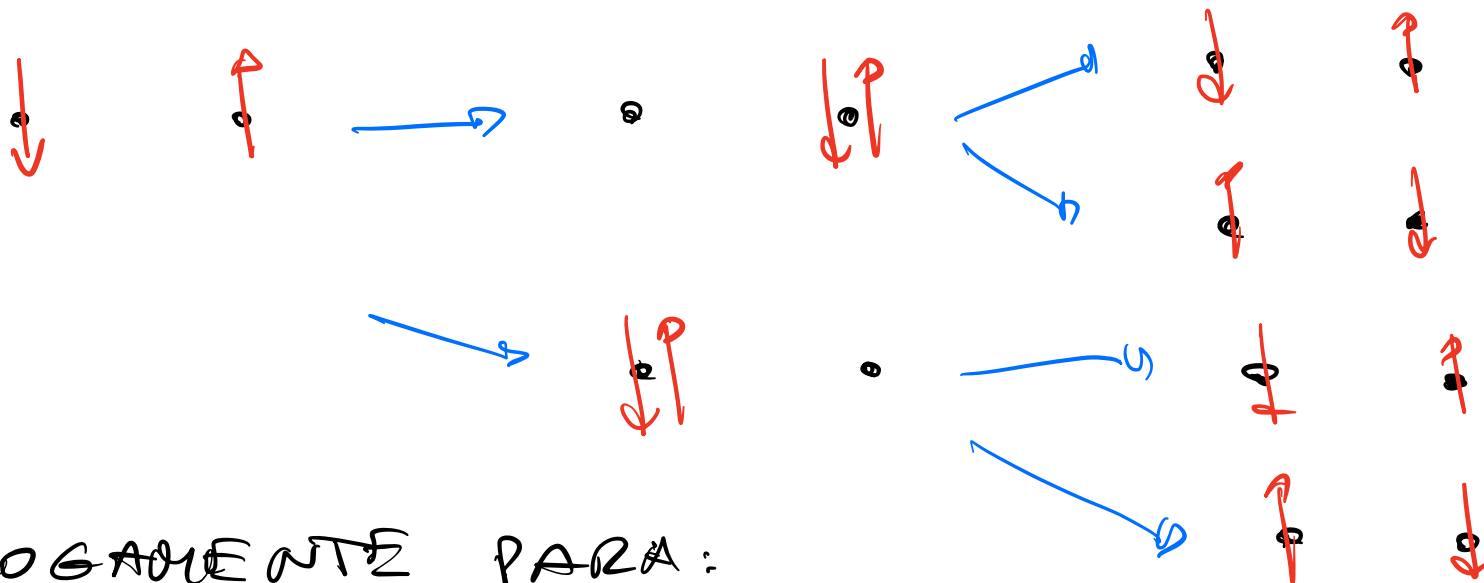
$$= -\frac{1}{U} \sum_m \langle \alpha | H_1 | m \rangle \langle m | H_2 | \beta \rangle$$

$$= -\frac{1}{U} \langle \alpha | H_1 \left(\underbrace{\sum_m |m\rangle \langle m|}_1 \right) H_2 | \beta \rangle$$

$$= -\frac{1}{U} \langle \alpha | H_2^2 | \beta \rangle$$

$$\langle \alpha | H_2^2 | \beta \rangle = t^2 \langle \alpha | \left(\sum_{\langle ij \rangle} (C_{i\sigma}^\dagger C_{j\sigma} + h.c.) \right) \left(\sum_{\langle mn \rangle} C_{m\sigma'}^\dagger C_{n\sigma'} + h.c. \right) | \beta \rangle$$

PARA CADA PAR DE SÍTIOS i E j :



ANALOGAMENTE PARA:



$$i=Q \quad \sum_{\sigma\sigma'} \langle \alpha | C_{i\sigma}^\dagger C_{j\sigma} C_{j\sigma'}^\dagger C_{i\sigma'} | \beta \rangle +$$

$$+ \sum_{\sigma\sigma'} \langle \alpha | C_{j\sigma}^\dagger C_{i\sigma} C_{i\sigma'}^\dagger C_{j\sigma'} | \beta \rangle =$$

$$= \sum_{\sigma\sigma'} \left[\langle \alpha | C_{i\sigma}^\dagger C_{i\sigma'} C_{j\sigma'}^\dagger C_{j\sigma} | \beta \rangle + \delta_{\sigma\sigma'} \langle \alpha | C_{i\sigma}^\dagger C_{i\sigma} | \beta \rangle \right.$$

$$\left. - \langle \alpha | C_{j\sigma}^\dagger C_{j\sigma'} C_{i\sigma'}^\dagger C_{i\sigma} | \beta \rangle + \delta_{\sigma\sigma'} \langle \alpha | C_{j\sigma}^\dagger C_{j\sigma} | \beta \rangle \right]$$

$$= - \sum_{\sigma\sigma'} \langle \alpha | C_{i\sigma}^\dagger C_{j\sigma'} C_{j\sigma'}^\dagger C_{i\sigma} | \beta \rangle + (i \leftrightarrow j)$$

$$+ \sum_{\sigma} \langle \alpha | C_{i\sigma}^\dagger C_{i\sigma} | \beta \rangle + (i \leftrightarrow j) \equiv X$$

2

$$A = \sum_{\sigma\sigma'} \langle \alpha | C_{i\sigma}^\dagger C_{i\sigma'} C_{j\sigma'}^\dagger C_{j\sigma} | \beta \rangle = \sum_{\substack{\alpha\beta \\ \lambda\mu}} (\delta_{\alpha\mu} \delta_{\beta\lambda}) C_{i\alpha}^\dagger C_{i\beta} C_{j\lambda}^\dagger C_{j\mu}$$

(NOTAS) $\delta_{\alpha\mu}\delta_{\beta\lambda} = \frac{1}{2} \left[\delta_{\alpha\beta}\delta_{\lambda\mu} + \sum_{a=1,2,3} \sigma_{\alpha\beta}^a \sigma_{\lambda\mu}^a \right]$

LEVANDO EM A:

$$A = \frac{1}{2} \sum_{\alpha\beta} C_{i\alpha}^\dagger C_{i\alpha} C_{j\beta}^\dagger C_{j\beta} + \frac{1}{2} \sum_{\substack{\alpha\beta \\ \lambda\mu \\ a}} (C_{i\alpha}^\dagger \sigma_{\alpha\beta}^a C_{i\beta}) (C_{j\lambda}^\dagger \sigma_{\lambda\mu}^a C_{j\mu})$$

$$X = 2 - \frac{1}{2} - \frac{1}{2} - \frac{1}{2} \times 2 \times 4 \vec{S}_i \cdot \vec{S}_j = 1 - 4 \vec{S}_i \cdot \vec{S}_j$$

ONDE: $\vec{S}_i \equiv \frac{1}{2} \sum_{\alpha\beta} C_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} C_{i\beta}$

POSSO PROVAR QUE: $[\vec{S}_i^a, \vec{S}_j^b] = \delta_{ij}(i) \epsilon^{abc} \vec{S}_i^c$

USANDO QUE $\sum_{\alpha} C_{i\alpha}^\dagger C_{i\alpha} = 1 \Rightarrow \vec{S}_i^2 = \frac{3}{4} \mathbb{1} \rightarrow$ ALGEBRA DE SPIN(1/2)

JUNTANDO TUDO:

$$H_{\text{sp}}^{(2)} = -\frac{J}{U} \times t^2 \sum_{\langle ij \rangle} [1 - 4 \vec{S}_i \cdot \vec{S}_j]$$

$$= \underbrace{\left(\frac{4t^2}{U} \right)}_J \sum_{\langle ij \rangle} \left[\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \right]$$

$$H^{(2)} = J \sum_{\langle ij \rangle} \left[\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \right] \rightarrow \text{HAMILTONIANO DE HEISENBERG}$$

PARA DOIS SÍTIOS:

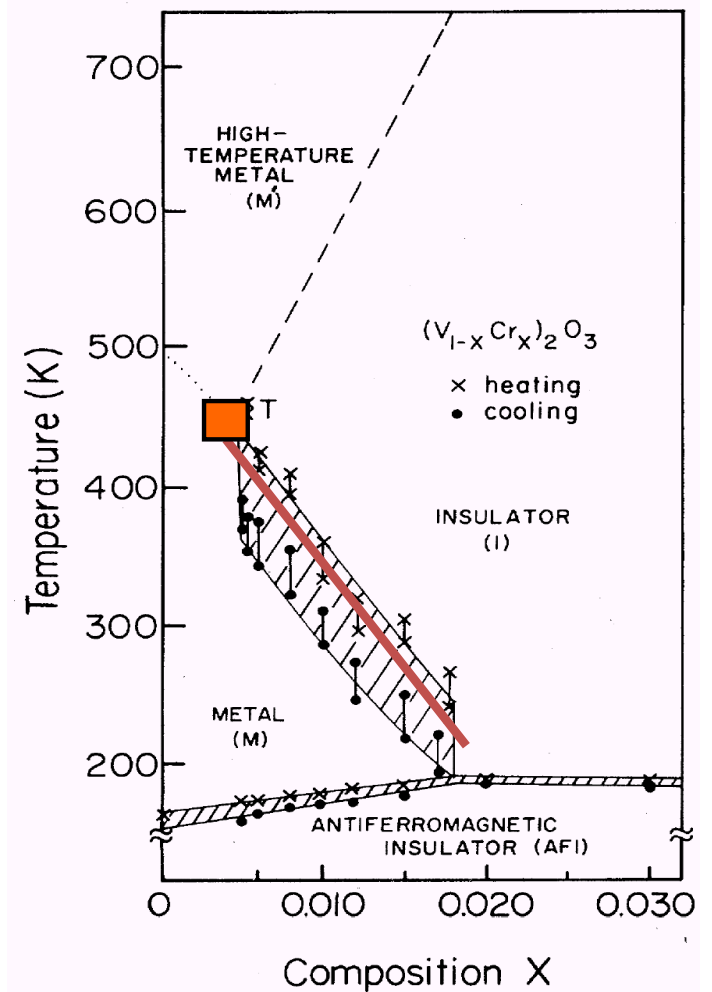
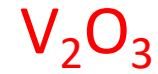
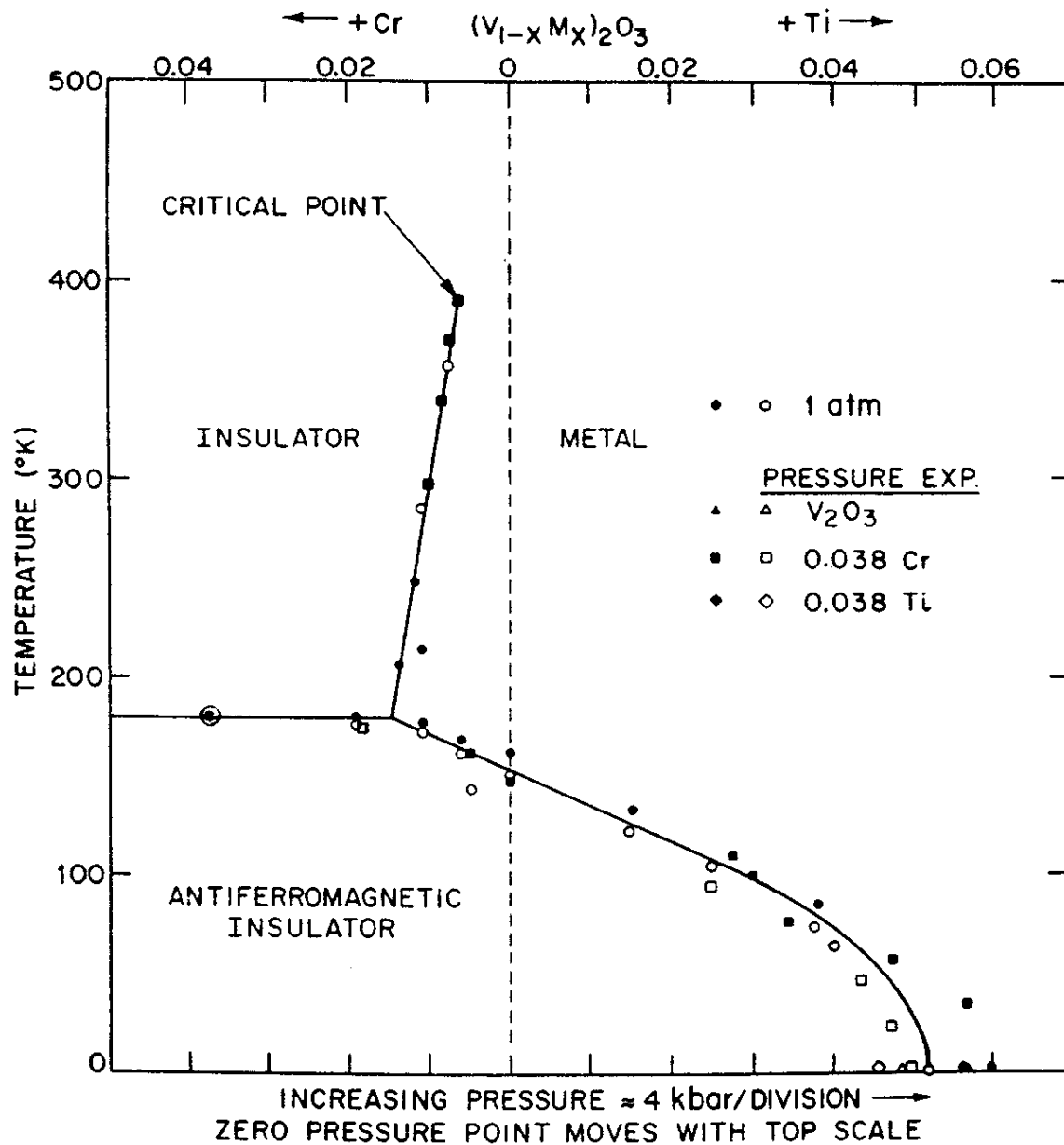
$$\boxed{J > 0}$$

$$\begin{aligned} J \vec{S}_1 \cdot \vec{S}_2 &= \frac{J}{2} \left[S_1^2 + S_2^2 - (S_1 - S_2)^2 \right] = \frac{J}{2} \left[S(S+1) - 2 \times \frac{3}{4} \right] \\ &= \frac{J}{2} S(S+1) - \frac{3}{4} J \end{aligned} \quad \begin{cases} S=0: & -\frac{3}{4} J \\ S=1: & \frac{1}{4} J \end{cases}$$

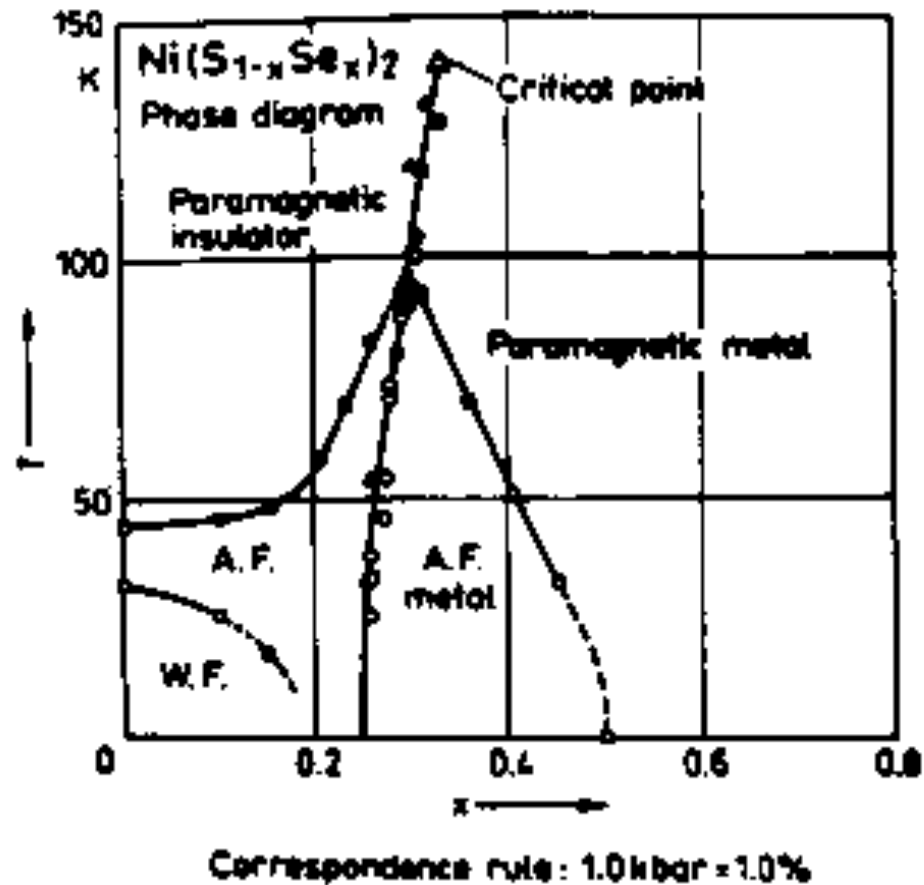
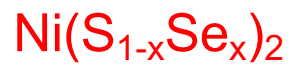
O MECANISMO ACIMA, QUE FAVORECE O
AFM É CONHECIDO COMO "SUPEREXCHANGE"

ANDERSON, P R (1953)

McWhan, D. B., A. Menth, J. P. Remeika, W. F. Brinkman, and T. M. Rice, 1973, Phys. Rev. B 7, 1920.



Kuwamoto, PRB '80



Czek *et al.*, JMMM 3, 58 (1976)

κ -(BEDT-TTF)₂Cu[N(CN)₂]Cl

