FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

1º Semestre de 2025
20/03/2025
Aula 7

Modelo de Hubbard

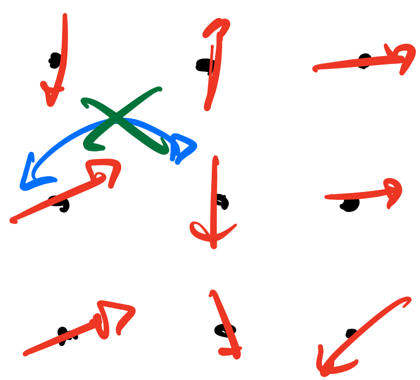
$$\boxed{H_{\text{Hubbard}} = \sum_{\mathbf{k}\sigma} \epsilon\left(\mathbf{k}\right) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{i\sigma} n_{i\uparrow} n_{i\downarrow}}$$

t

Transição metal-isolante de Mott-Hubbard em semi-preenchimento: $n = \frac{N}{N_s} = 1$

$t \gg U$: METAL

$t \ll U$:



ISOLANTE DE MOTT-HUBBARD

$\left(\frac{U}{t}\right)_c \longrightarrow$ TRANSIÇÃO METAL-ISOLANTE

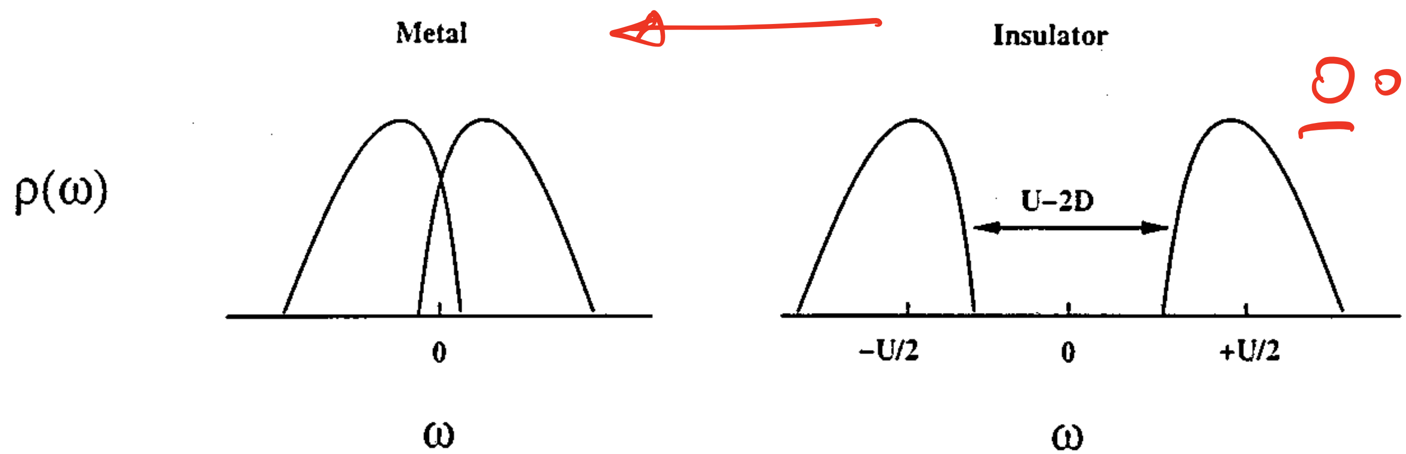
$\left(\frac{U}{t}\right)_c = 0$ EM 1D (LIEB + WU)

Primeiras descrições teóricas

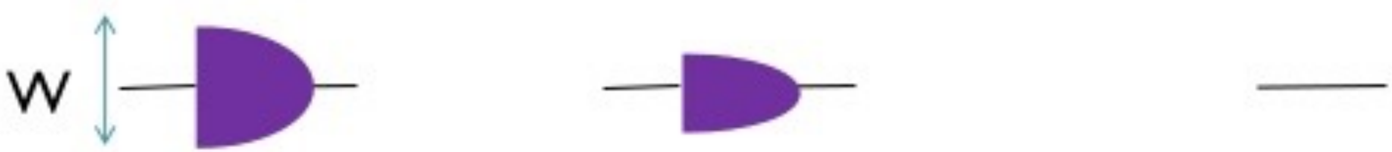
- A descrição de Hubbard III: do isolante para o metal; duas bandas (de Hubbard) separadas que se tocam na transição (J. Hubbard, Proc. R. Soc. (London) A **281**, 401 (1964))

↑ ou ↓ → $-\frac{U}{2}$

0 ou 2 → $\frac{U}{2}$



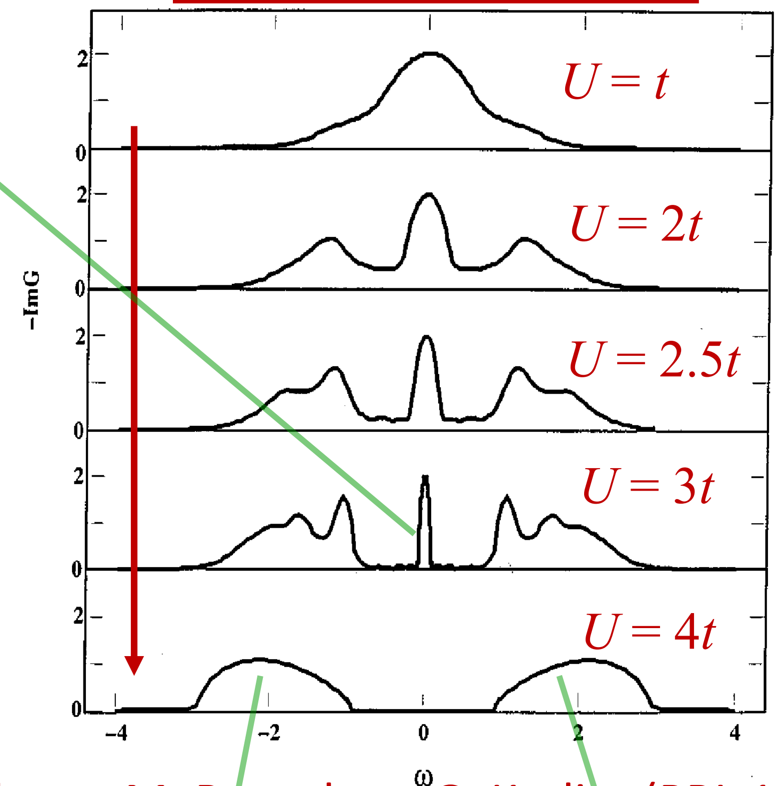
- A descrição de Brinkman e Rice: do metal para o isolante; desaparecimento das quasi-partículas, $m^* \to \infty$; não há bandas de Hubbard (W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970))



Teoria dinâmica de campo médio (Dynamical mean field theory)

Pico de quasi-partículas (Brinkman-Rice)

Density of states

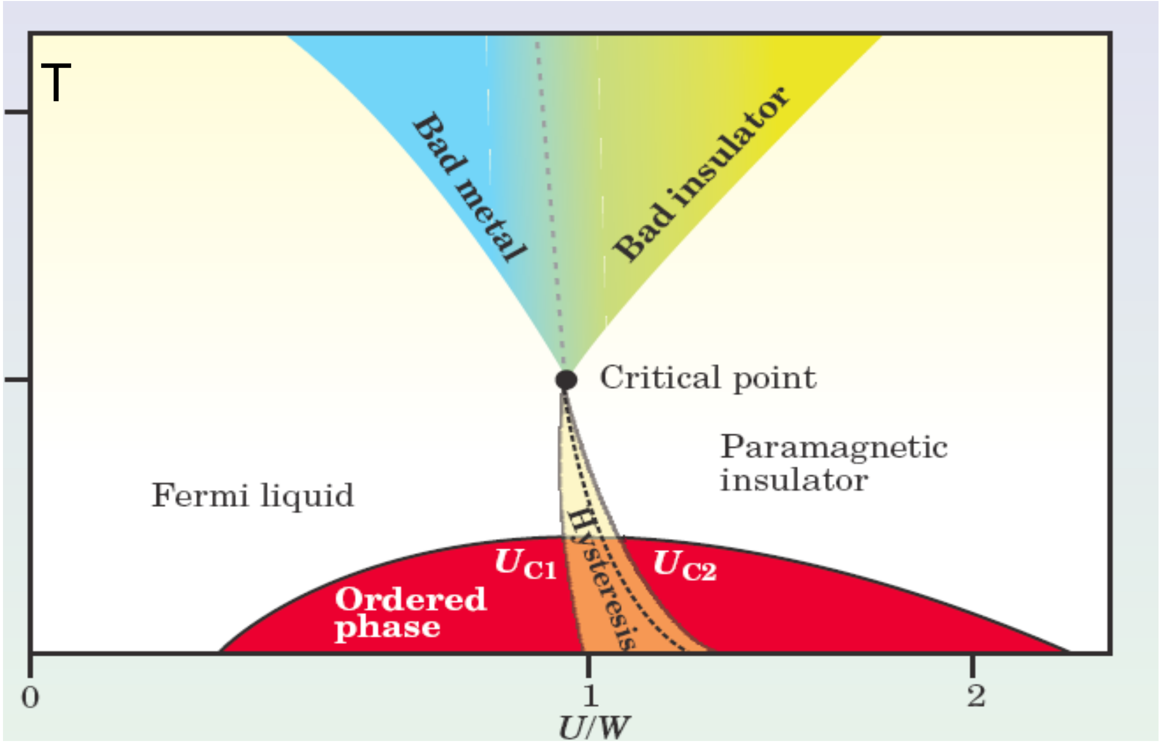


Unificação de Brinkman-Rice + Hubbard III

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

Bandas de Hubbard (Hubbard III)

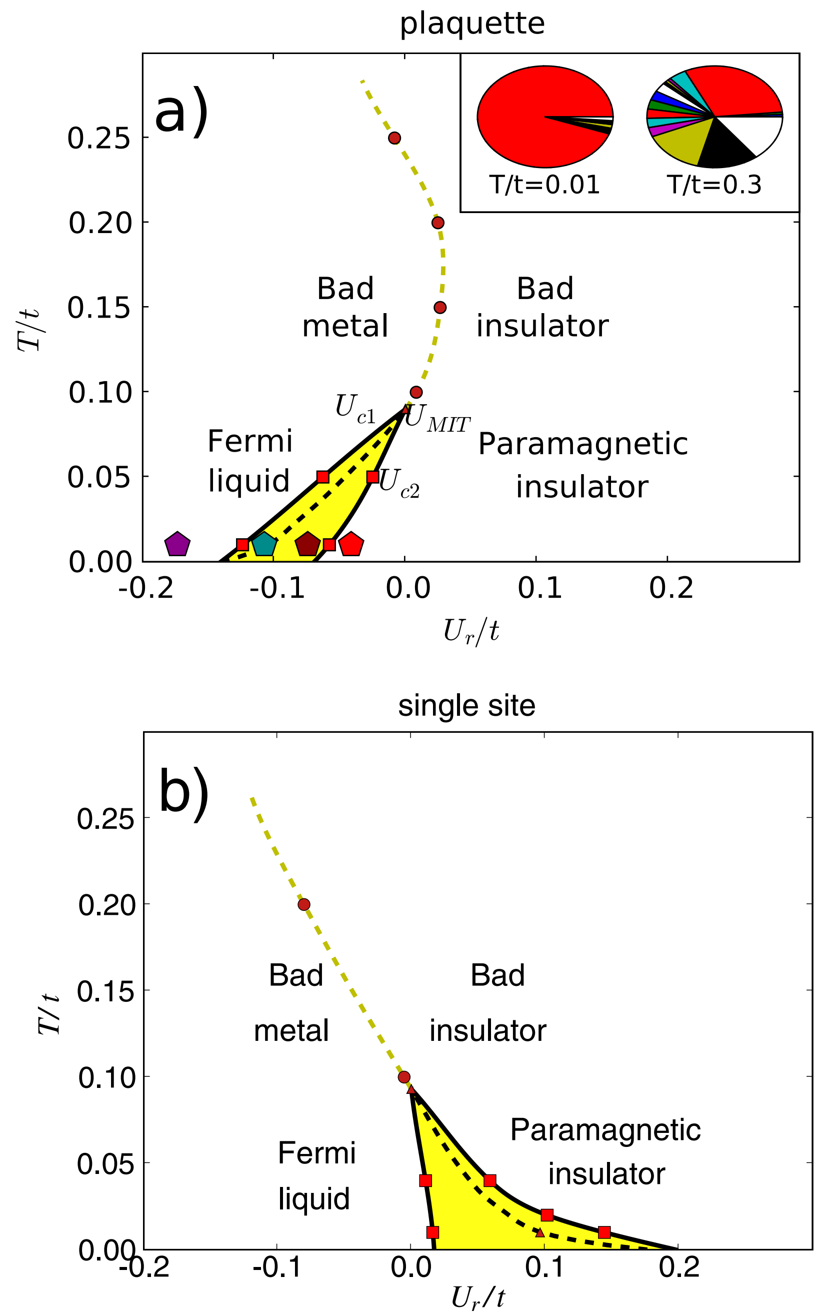
Diagrama de fases (DMFT)



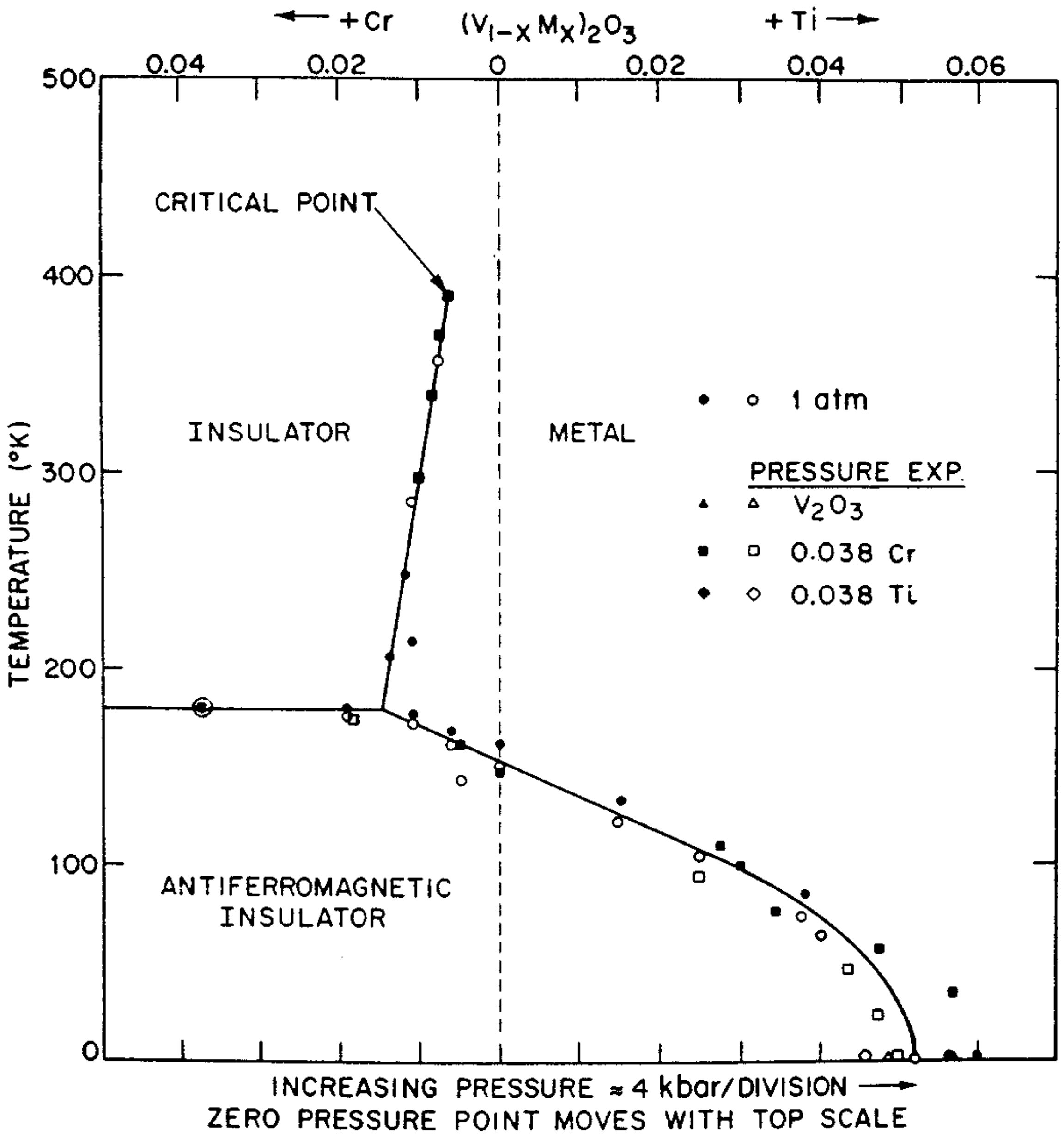
Kotliar, Vollhardt, Phys. Today (2004)

Além da DMFT: cluster DMFT

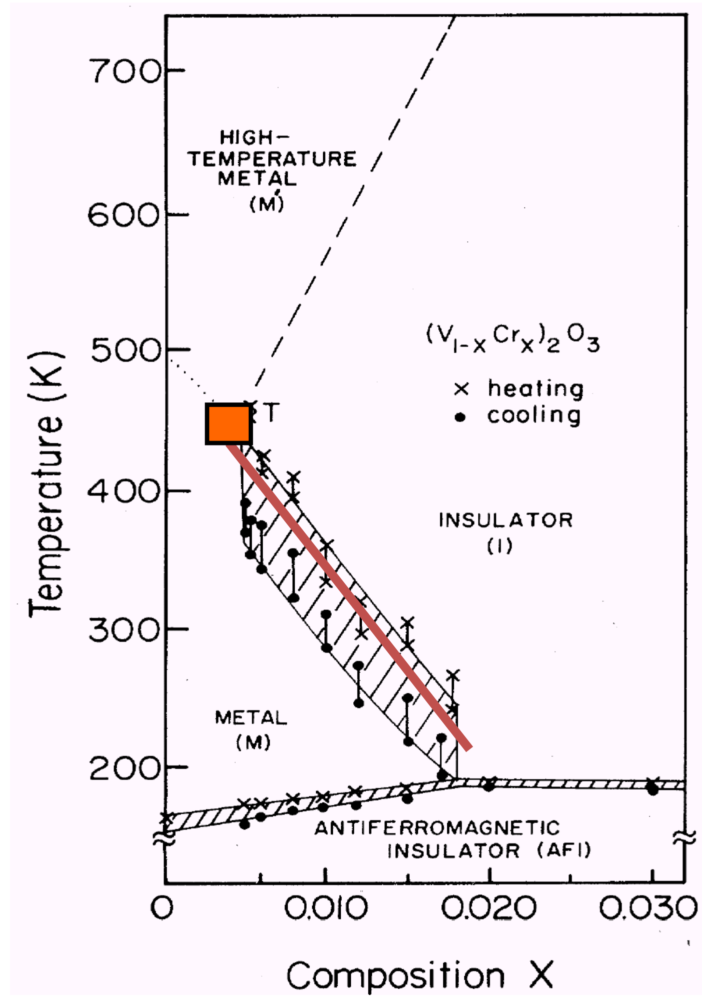
H. Park, K. Haule, and G. Kotliar
Phys. Rev. Lett. **101**, 186403 (2008).



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



V_2O_3

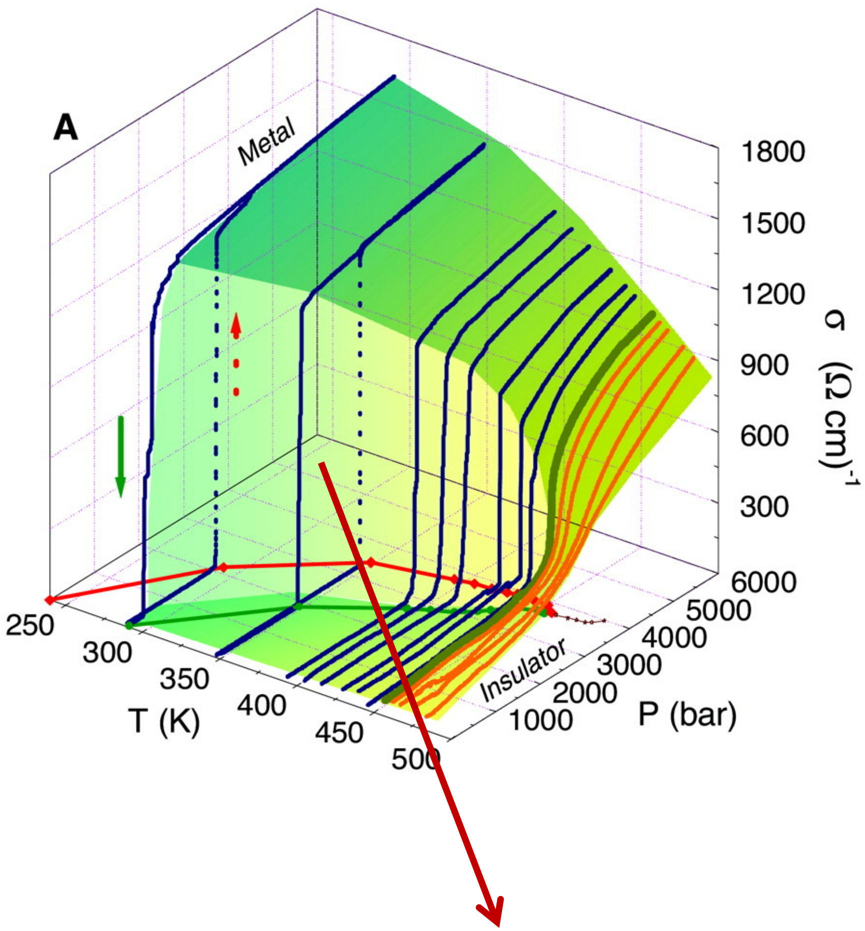


Kuwamoto, PRB '80

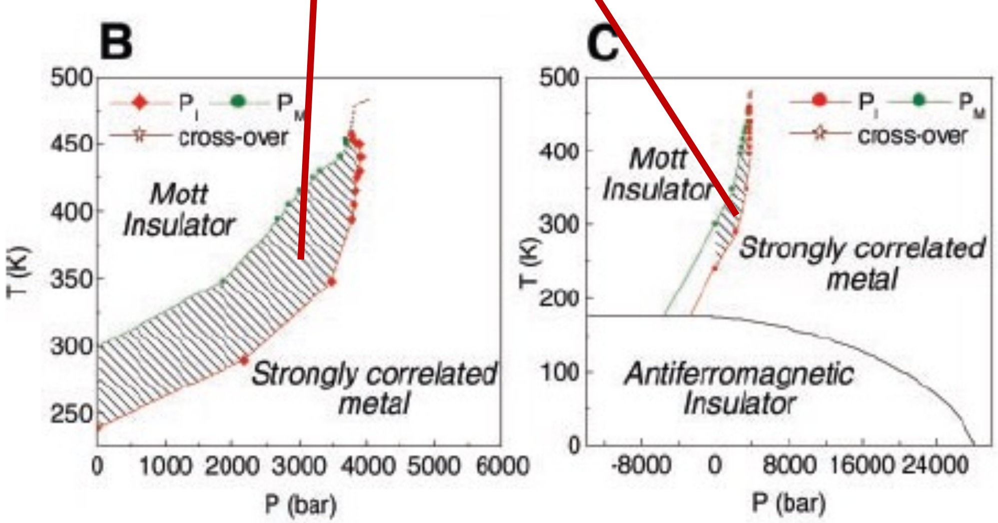
- Pressão aumenta t, diminui U/t, favorece o comportamento metálico.
- Pressão química: elemento de raio iônico maior/menor aumenta o parâmetro de rede e age como pressão negativa/positiva.

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

$(V_{0.989}Cr_{0.011})_2O_3$



Coexistência metal-isolante



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

$Ni(S_{1-x}Se_x)_2$

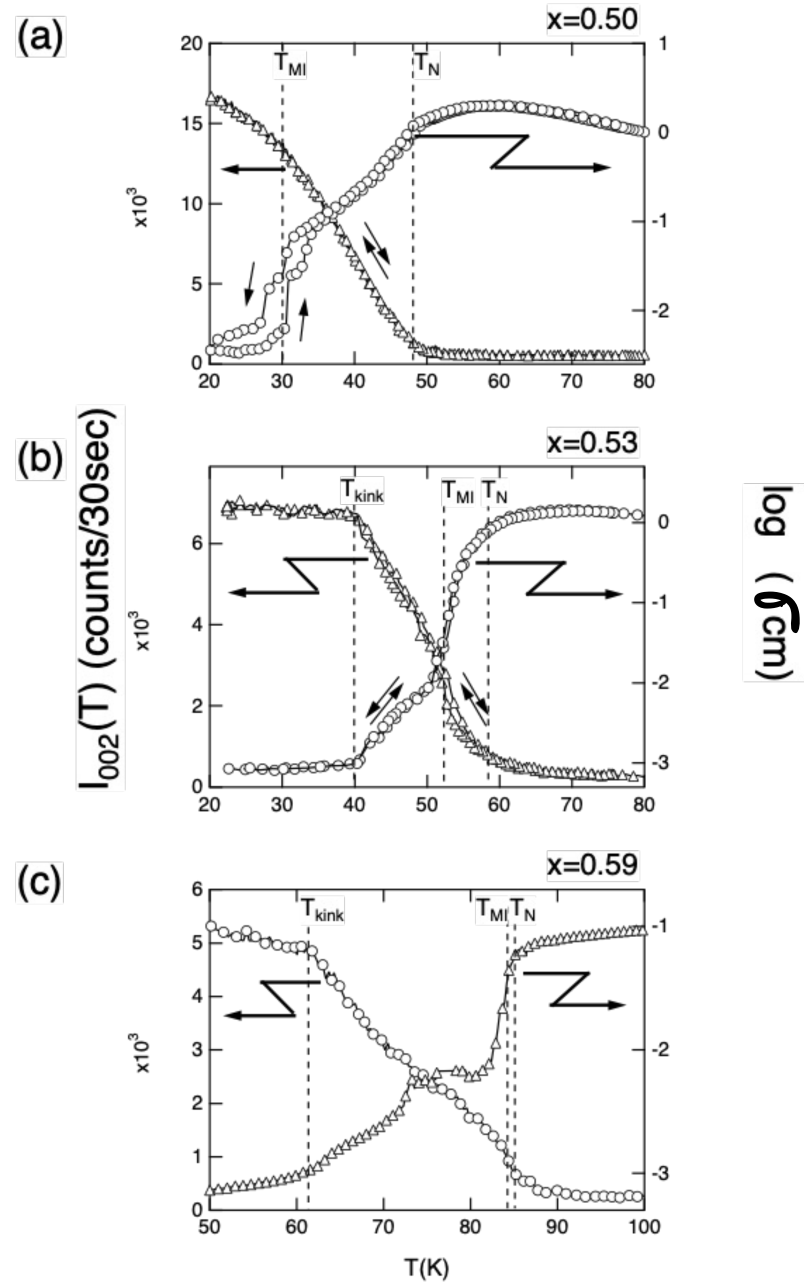
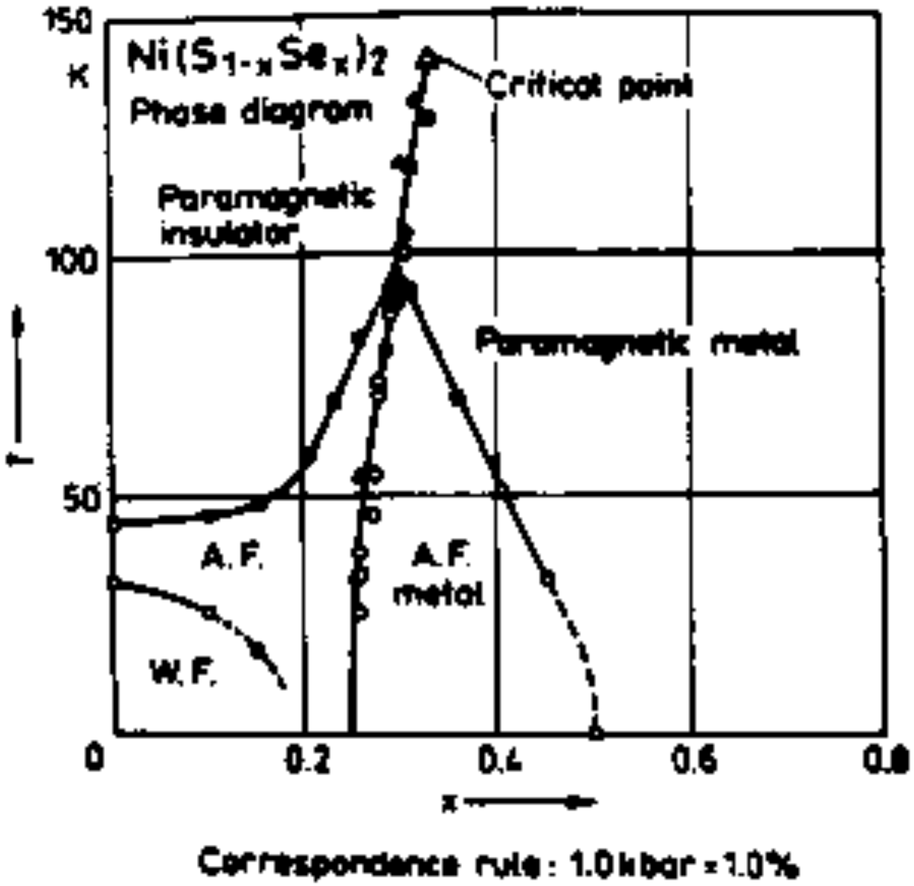


Fig. 5. Temperature dependences of the electrical resistivity and the peak intensity of (002) antiferromagnetic Bragg reflection, $I_{002}(T)$ measured simultaneously for (a) $x = 0.50$ and (b) $x = 0.53$, and separately for (c) $x = 0.59$. Circles and triangles indicate electrical resistivity and $I_{002}(T)$,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

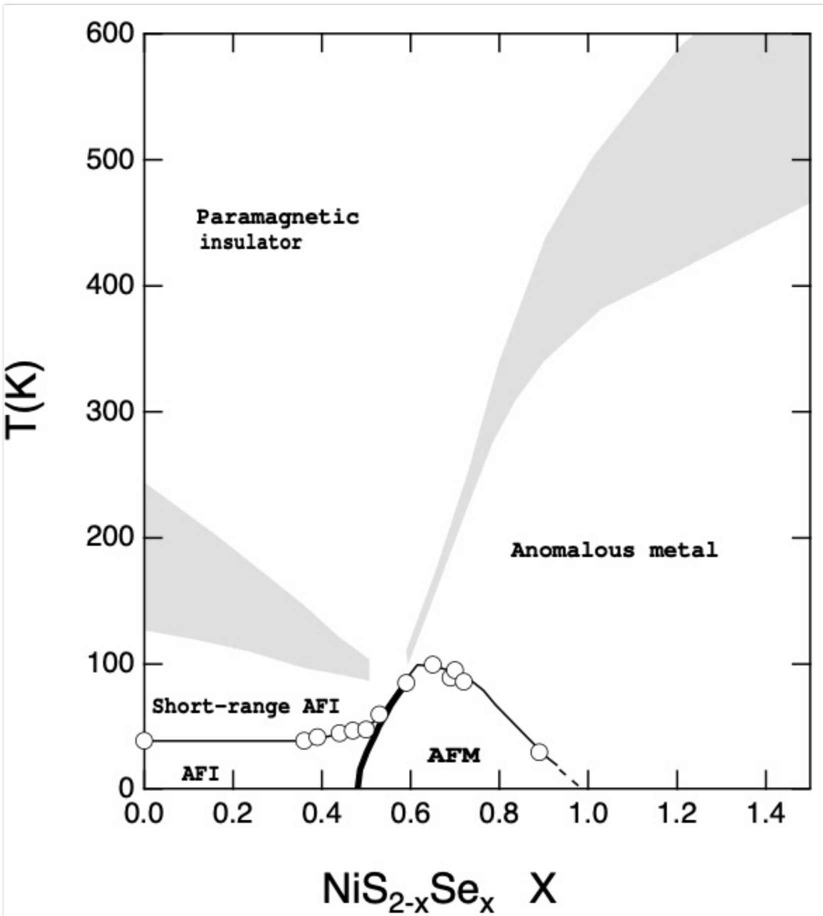
M. Matsuura *et al.,* J. Phys. Soc. Jpn **69**, 1503 (2000)

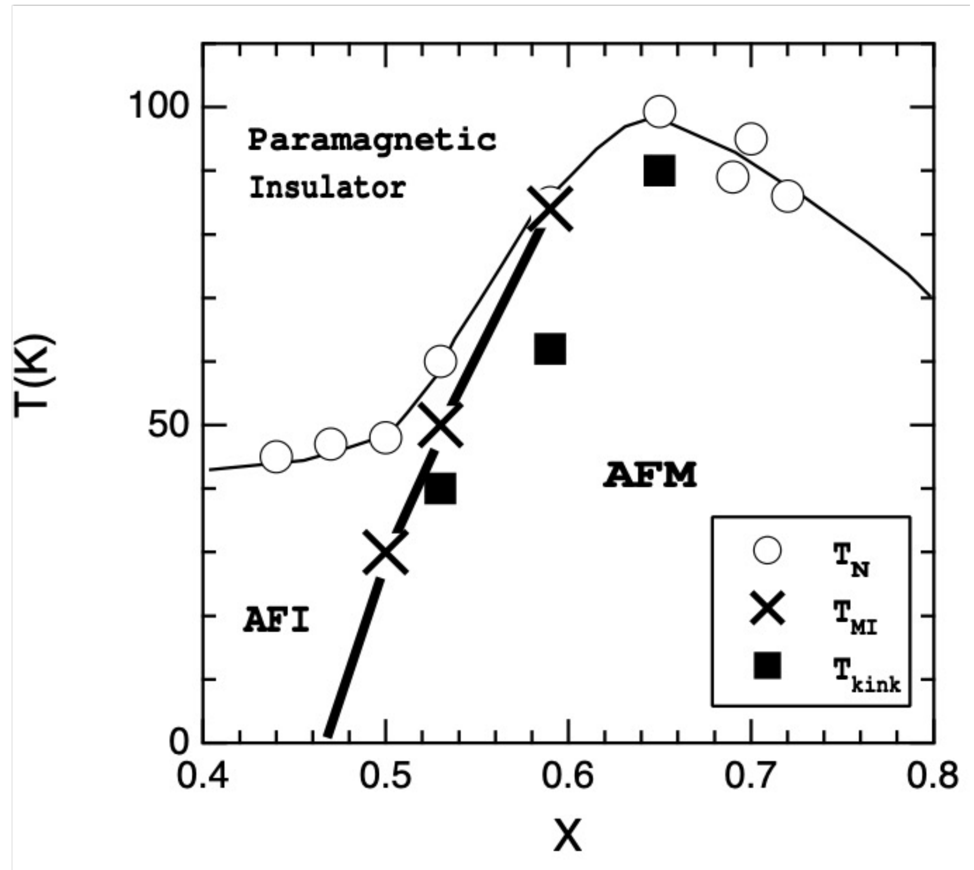
$Ni(S_{1-x}Se_x)_2$



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

$Ni(S_{1-x}Se_x)_2$

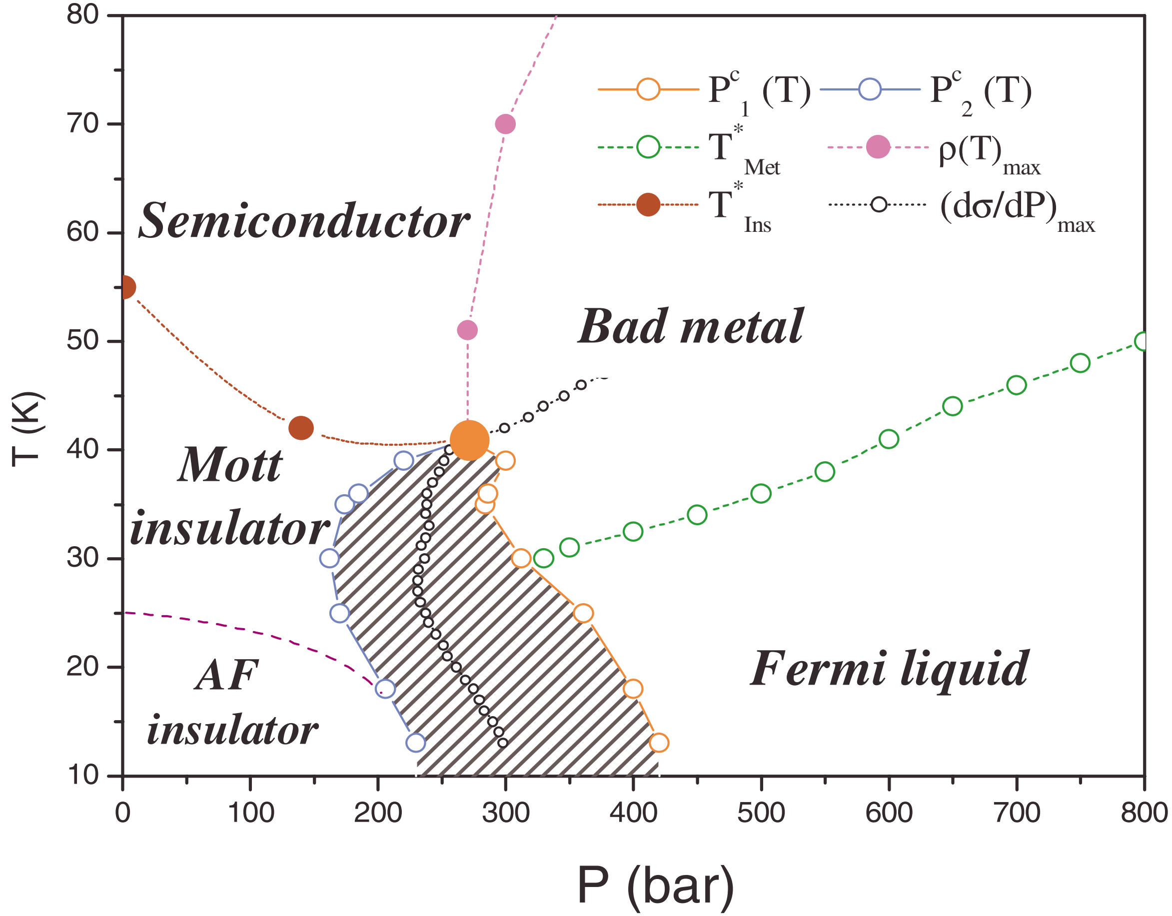




M. Matsuura *et al.,* J. Phys. Soc. Jpn **69**, 1503 (2000)

Condutores orgânicos fortemente bi-dimensionais

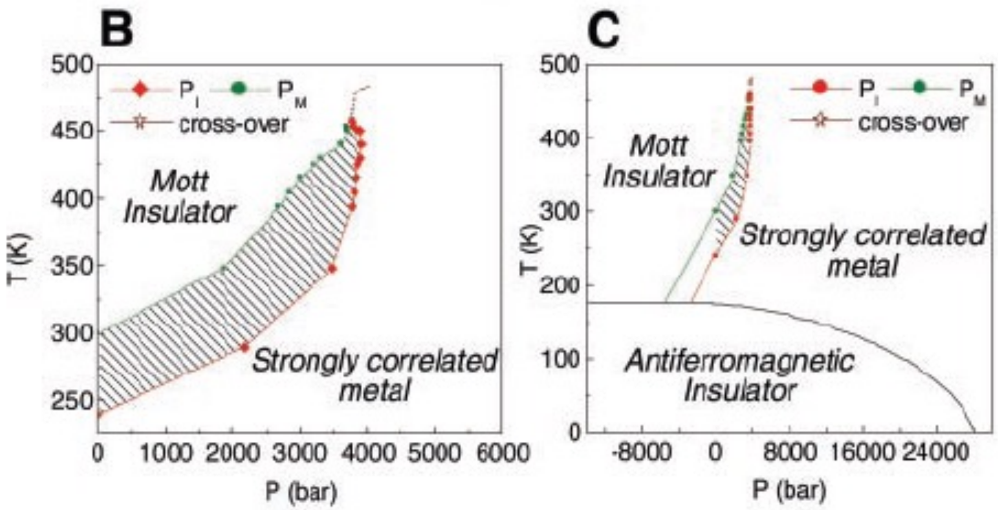
$\kappa\text{-(BEDT-TTF)}_2\text{Cu[N(CN)}_2\text{]Cl}$

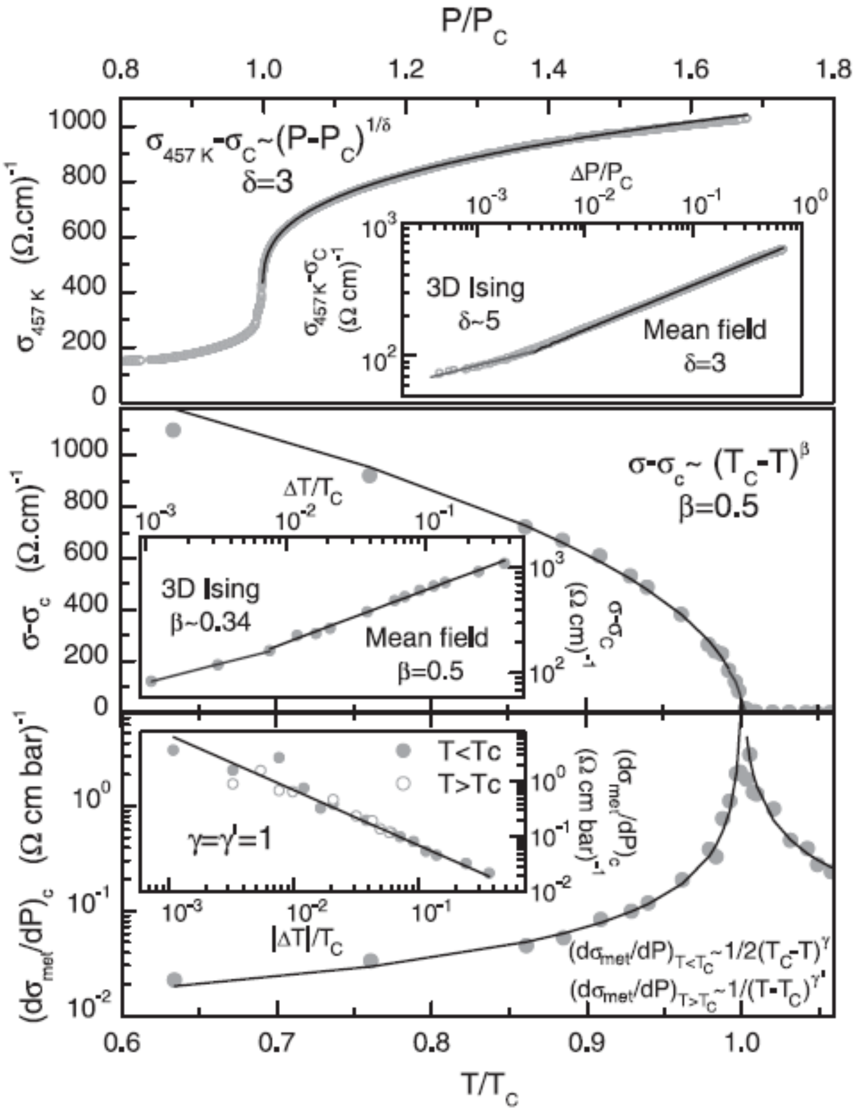


Transição de Mott: o ponto crítico

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

$(V_{0.989}Cr_{0.011})_2O_3$

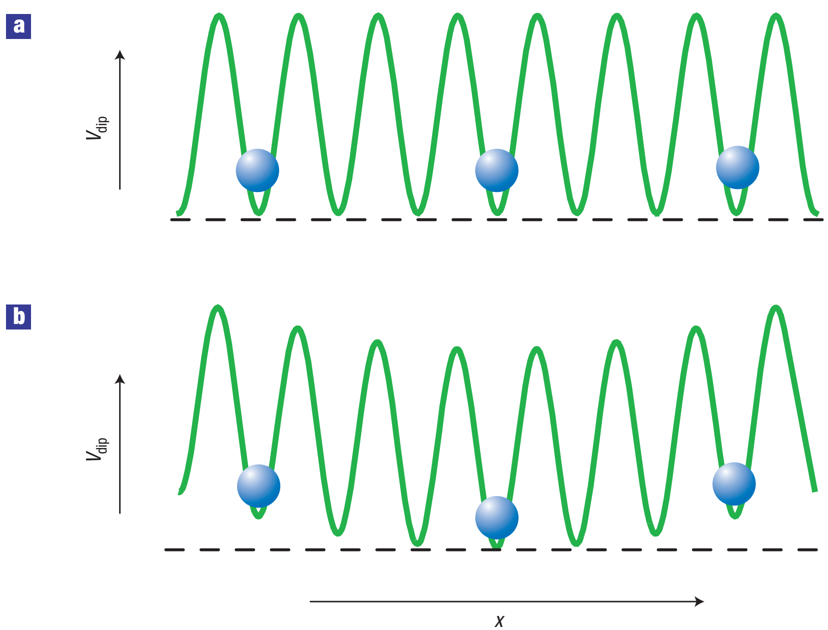


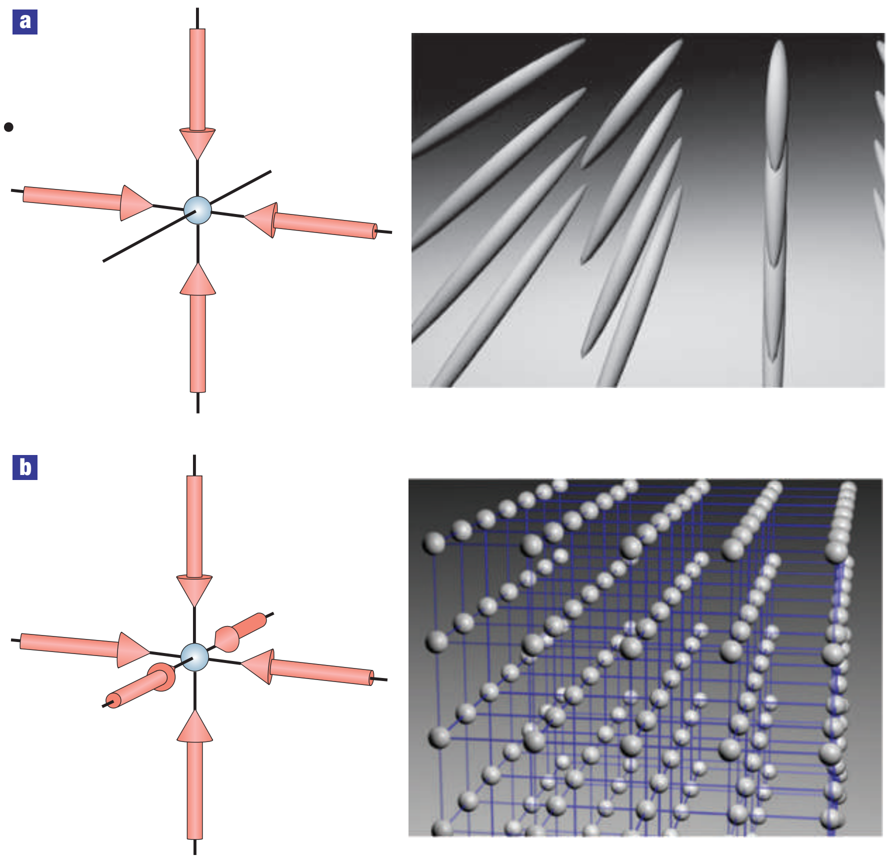


O modelo de Hubbard para átomos frios: redes ópticas

$\vec{d} = \alpha \vec{E}$

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





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

Modelo de Bose-Hubbard

MODELO PARA BÓSONS DE SPIN $S=0$

$$H_{BH} = -t \sum_{\langle i,j \rangle} \left(b_i^\dagger b_j + h.c. \right) + \frac{U}{2} \sum_i \left(b_i^\dagger b_i^\dagger b_i b_i \right)$$

$$b_i^\dagger \underbrace{b_i^\dagger b_i}_{} b_i = b_i^\dagger \left(b_i b_i^\dagger - 1 \right) b_i = b_i^\dagger b_i b_i^\dagger b_i - b_i^\dagger b_i$$

$$b_i b_i^\dagger - b_i^\dagger b_i = 1$$

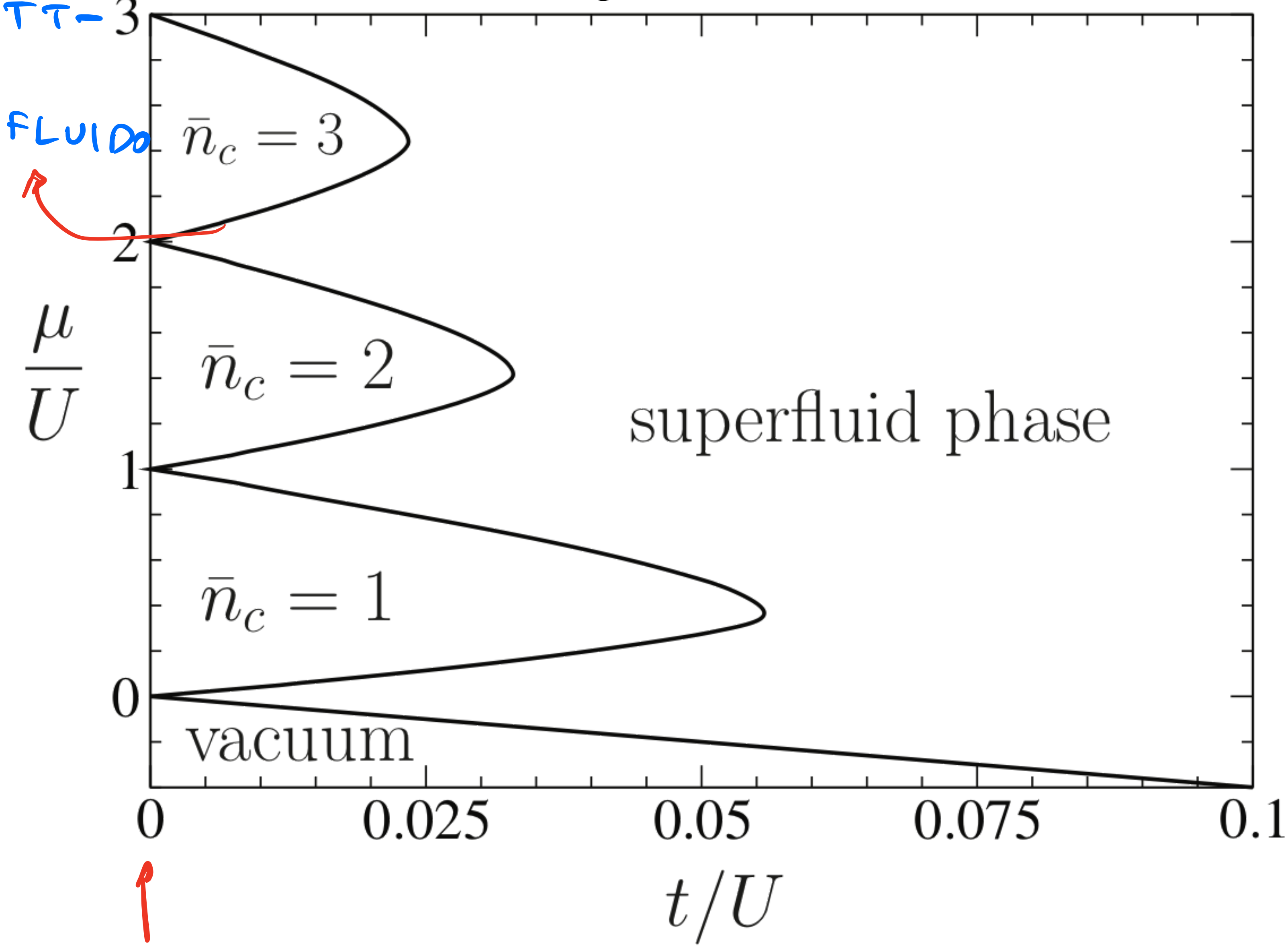
$$\hat{n}_i = b_i^\dagger b_i \Longrightarrow \frac{U}{2} \sum_i \left(\hat{n}_i \hat{n}_i - \hat{n}_i \right) = \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right)$$

$$H_{BH} = -t \sum_{\langle i,j \rangle} \left(b_i^\dagger b_j + h.c. \right) + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right)$$

Diagrama de fases

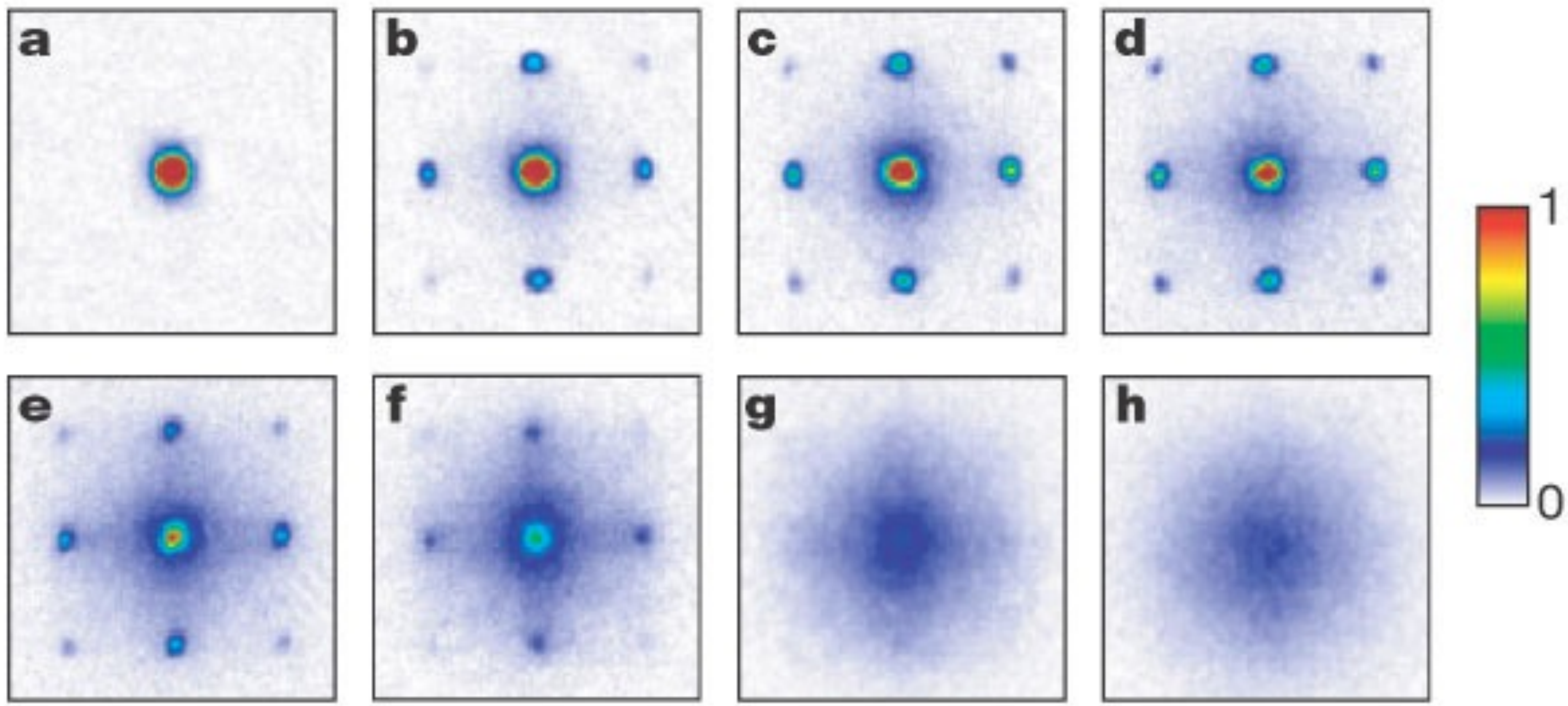
TRANSIÇÃO ISOLANTE T=0
DE MOTT-

SUPERFLUIDO



$U = \infty$

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



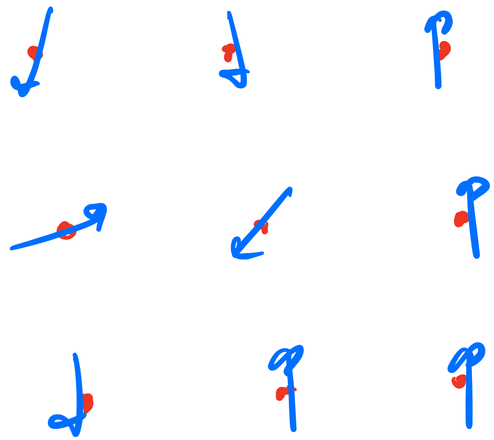
Markus Greiner *et al.*, Nature **415**, 39 (2002)

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

SEMI-PREENCHIMENTO ($n=1$) E $U \gg t$ (ISOLANTE DE MOTT)



DEGENER.

2^{N_s}

TEORIA DE PERTURBAÇÃO EM t:

$$H_0 = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$H_1 = -t \sum_{\substack{\langle ij \rangle \\ \sigma}} \left(c^\dagger_{i\sigma} c_{j\sigma} + h.c. \right)$$

T.P. DEGENERADA: EST. FUND.: $|\alpha\rangle = |\sigma_1, \sigma_2, \dots \sigma_{N_s}\rangle$

PRIMEIRA ORDEM: $M_{\alpha\beta} = \langle \alpha | H_1 | \beta \rangle$

$$= -t \sum_{\substack{\langle ij \rangle \\ \sigma}} \langle \alpha | \left(c^\dagger_{i\sigma} c_{j\sigma} + h.c. \right) | \beta \rangle$$

$H_1 \rightarrow$ CRIA UMA VACÂNCIA E UMA DUPLA OCUPAÇÃO

$\Rightarrow M_{\alpha\beta} = 0$

EM SEGUNDA ORDEM:

$$H^{(2)}_{\alpha\beta} = \sum_{n\neq 0} \frac{\langle \alpha | H_1 | n \rangle \langle n | H_1 | \beta \rangle}{E_0^{(0)} - E_n^{(0)}}$$

$E_0^{(0)} = 0$

ESTADOS EXC. $|n\rangle \rightarrow$ 1 VACÂNCIA E 1 DUPLA OCUPAÇÃO

$E_n^{(0)} = U$

$$H^{(2)}_{\alpha\beta} = -\frac{1}{U} \sum_{n\neq 0} \langle \alpha | H_1 | n \rangle \langle n | H_1 | \beta \rangle$$

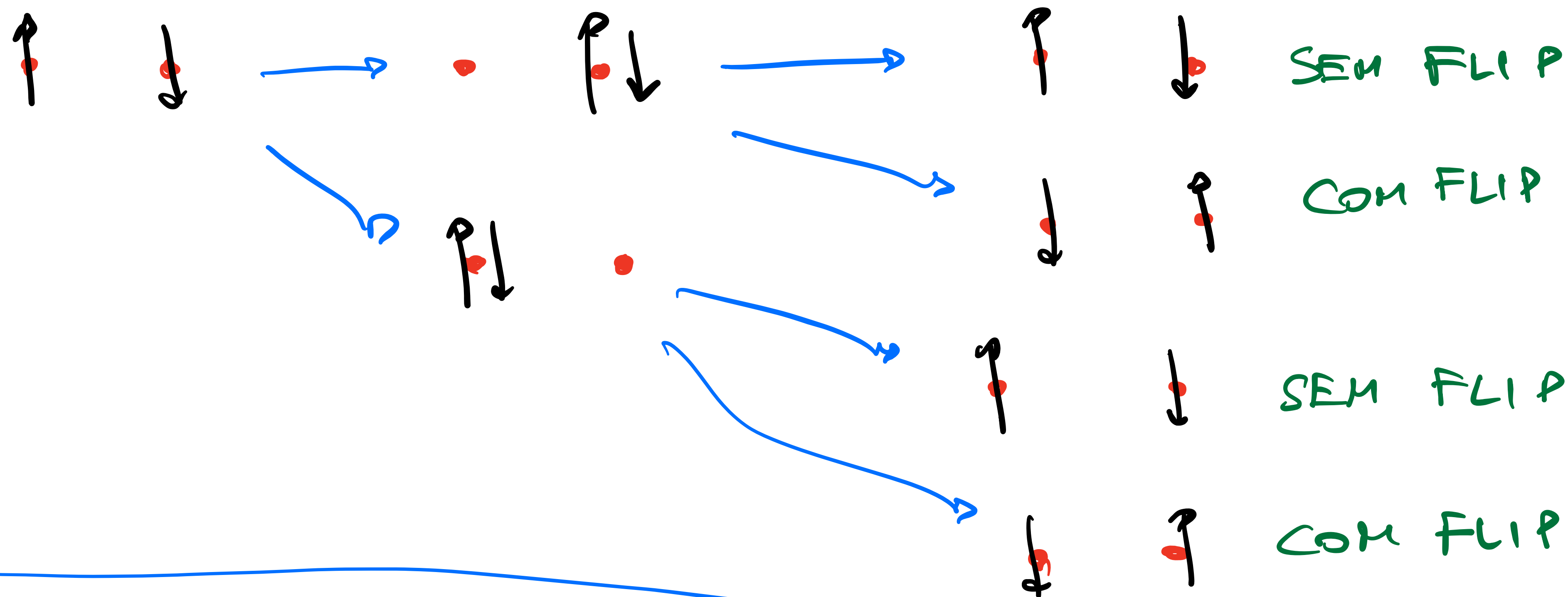
MAS: $\mathbb{1} = \sum_{\gamma} |\gamma\rangle\langle\gamma| + \sum_{n\neq 0} |n\rangle\langle n|$

$$H^{(2)}_{\alpha\beta} = -\frac{1}{U} \langle \alpha | H_1 \Big[\mathbb{1} - \sum_{\gamma} \cancel{|\gamma\rangle\langle\gamma|} \Big] H_1 | \beta \rangle$$

$$= -\frac{1}{U} \langle \alpha | H_1^2 | \beta \rangle$$

$$H^{(2)}_{\alpha\beta} = -\frac{t^2}{U} \sum_{\substack{ij\\ \sigma}} \sum_{\substack{\ell, m\\ \sigma'}} \langle \alpha | (c^\dagger_{i\sigma} c_{j\sigma} + h.c.)(c^\dagger_{\ell\sigma'} c_{m\sigma'} + h.c.) | \beta \rangle$$

PARA CADA PAR DE SÍTIO, O 1º OPERADOR TRANSFERE UM ELÉTRON DE UM SÍTIO PRO VIZINHO, ASSIM CRIANDO UMA VACÂNCIA E UMA DUPLA OC., E O 2º OPERADOR FAZ O INVERSO TRAZENDO DE VOLTA À VARIEDADE DE $|\alpha\rangle$.



SEMELHANTEMENTE PARA: ↓ ↑

MAS NOTE QUE PARA: ↑ ↑ OU ↓ ↓

NÃO HÁ PROCESSO POSSÍVEL.

CLARAMENTE, OS PROCESSOS PERMITIDOS, POR ABAIXAREM A ENERGIA, FAVORECEM A CONFIGURAÇÃO ANTI-PARALELA

CONTANDO TODOS OS PROCESSOS E GARANTINDO O SINAL, OBTEMOS:

$$H_H = \sum_{\langle i,j \rangle} \underbrace{\left(\frac{4t^2}{U}\right)}_{J} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4}\right) = J \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4}\right)$$

PARA CADA PAR: $|S=0, M=0\rangle = |0,0\rangle$ (SINGLETO)

$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

$$|1,0\rangle = |S=1, M=0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$

$$|1,1\rangle = |S=1, M=+1\rangle = |\uparrow\uparrow\rangle$$

$$|1,-1\rangle = |S=1, M=-1\rangle = |\downarrow\downarrow\rangle$$

$$(\vec{S}_i \cdot \vec{S}_j - \tfrac{1}{4})|0,0\rangle = (-\tfrac{3}{4} - \tfrac{1}{4})|0,0\rangle = -|0,0\rangle$$

$$(\vec{S}_i \cdot \vec{S}_j - \tfrac{1}{4})|1,m\rangle = (\tfrac{1}{4} - \tfrac{1}{4})|0,0\rangle = 0$$

ESQUECENDO A CONSTANTE:

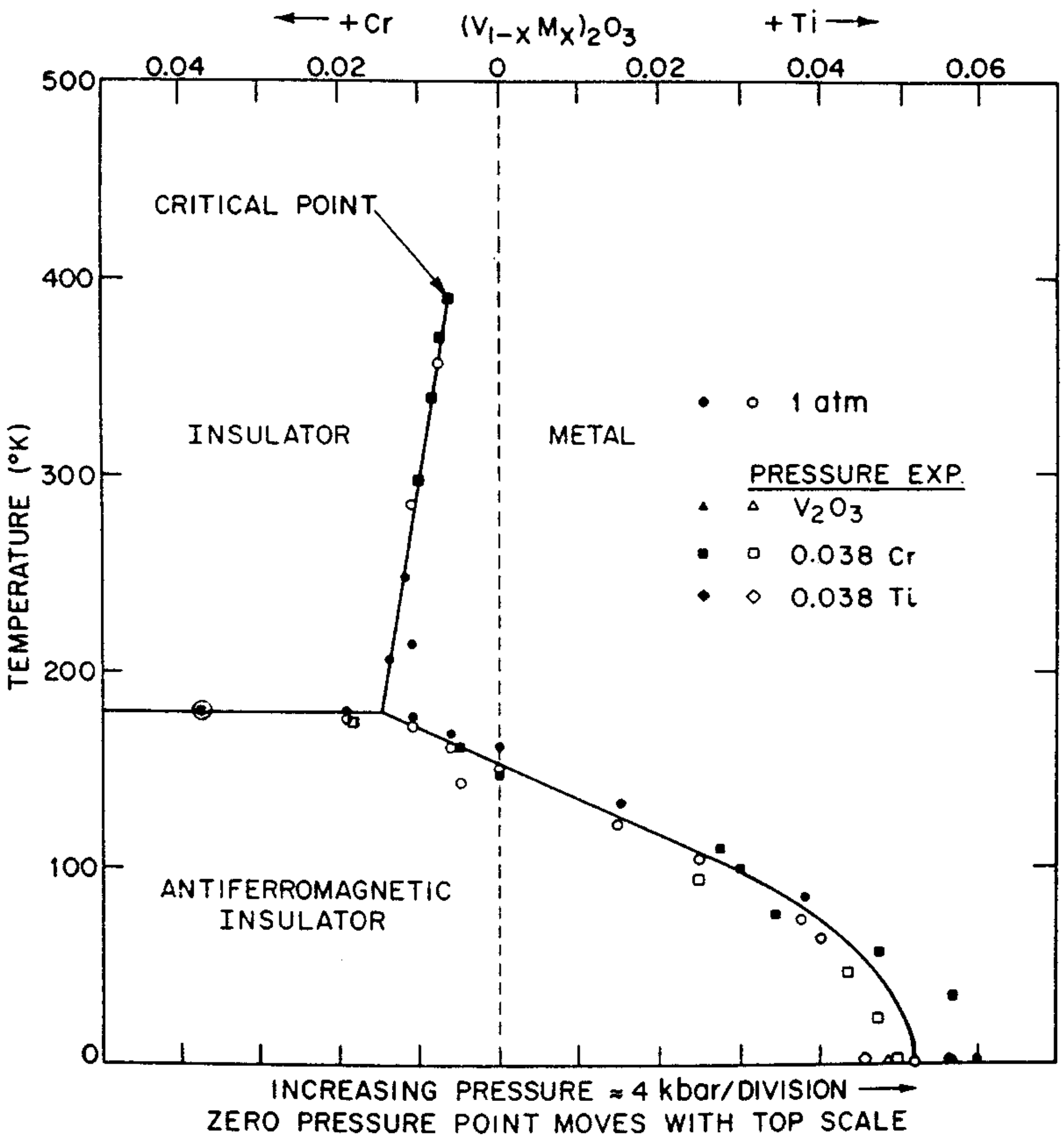
$$\boxed{H_H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j} \qquad J > 0$$

SUPER-EXCHANGE (ANDERSON, 1959)

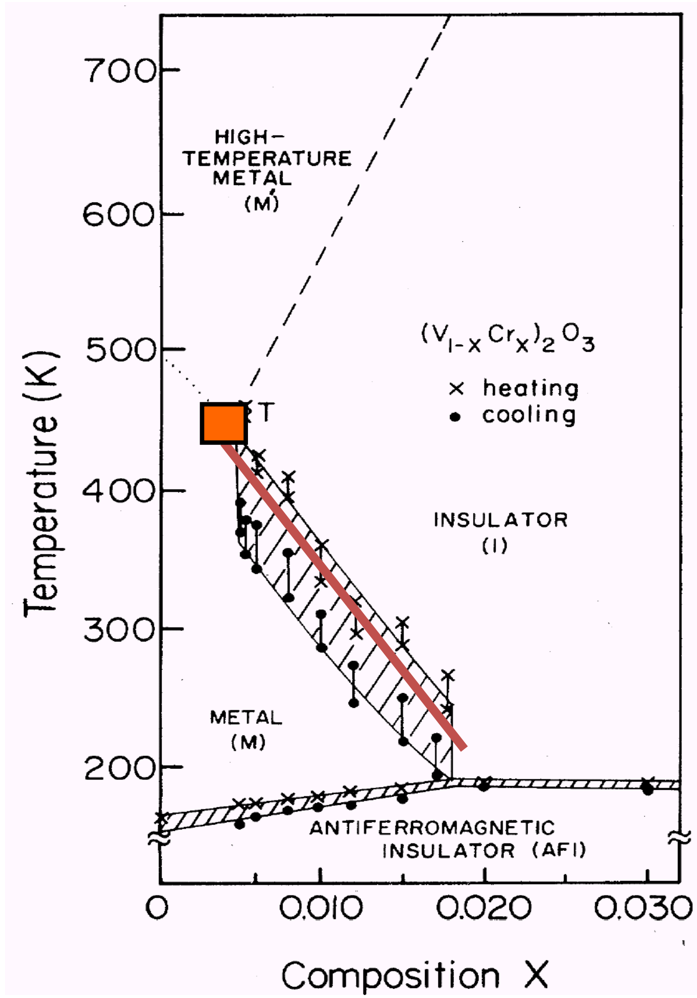
O modelo de Heisenberg

$$\boxed{\begin{gathered} H = J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \right) \\ J = \frac{4t^2}{U} \end{gathered}}$$

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

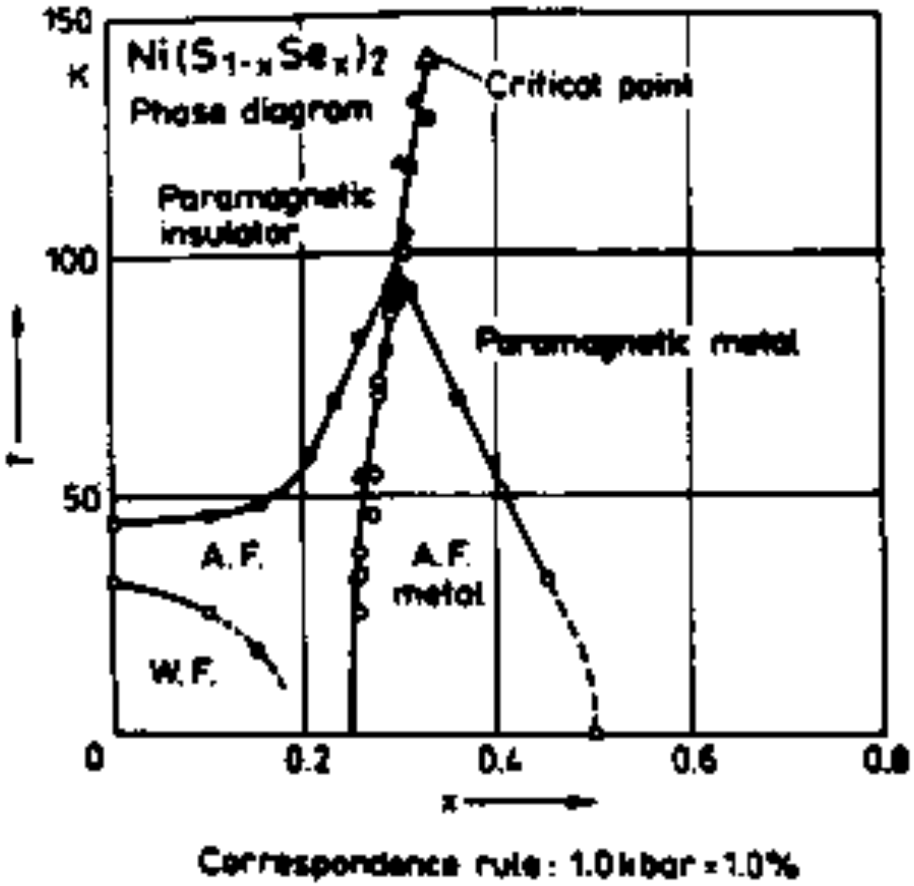


V_2O_3

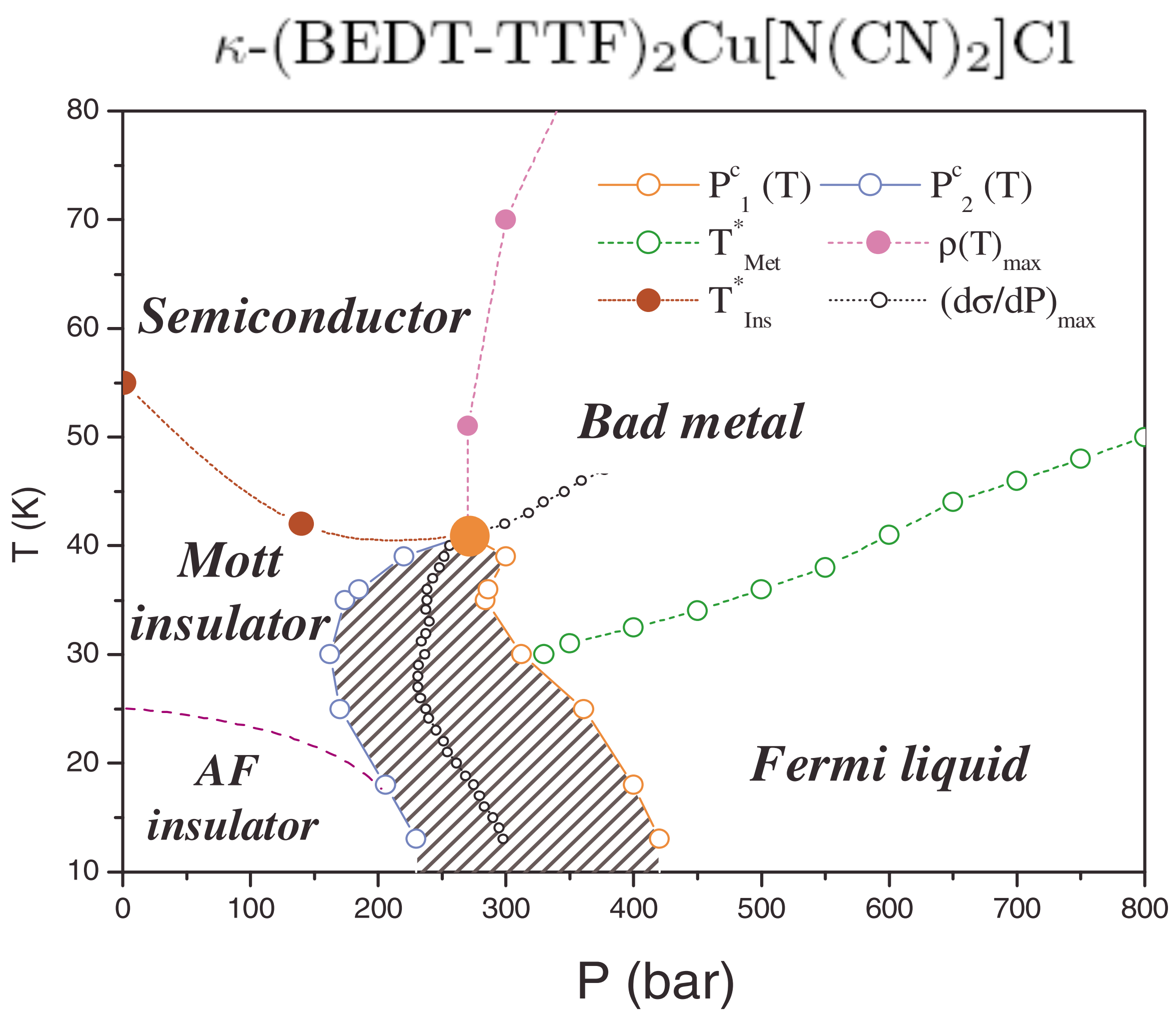


Kuwamoto, PRB '80

$Ni(S_{1-x}Se_x)_2$



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


κ-(BEDT-TTF)2Cu[N(CN)2]Cl
P^c_1 (T)
P^c_2 (T)
T*Met
ρ(T)max
T*Ins
(dσ/dP)max
Semiconductor
Bad metal
Mott insulator
AF insulator
Fermi liquid
T (K)
P (bar)
80
70
60
50
40
30
20
10
0
100
200
300
400
500
600
700
800