FI 193 – Teoria Quântica de Sistemas de Muitos Corpos

2º Semestre de 2023

29/08/2023

Aula 8

O modelo de Heisenberg

MODELO DE HUBBARD EM SEMI-PREENCHIMENTO $n=1$, NO LIMITE $U \gg t$

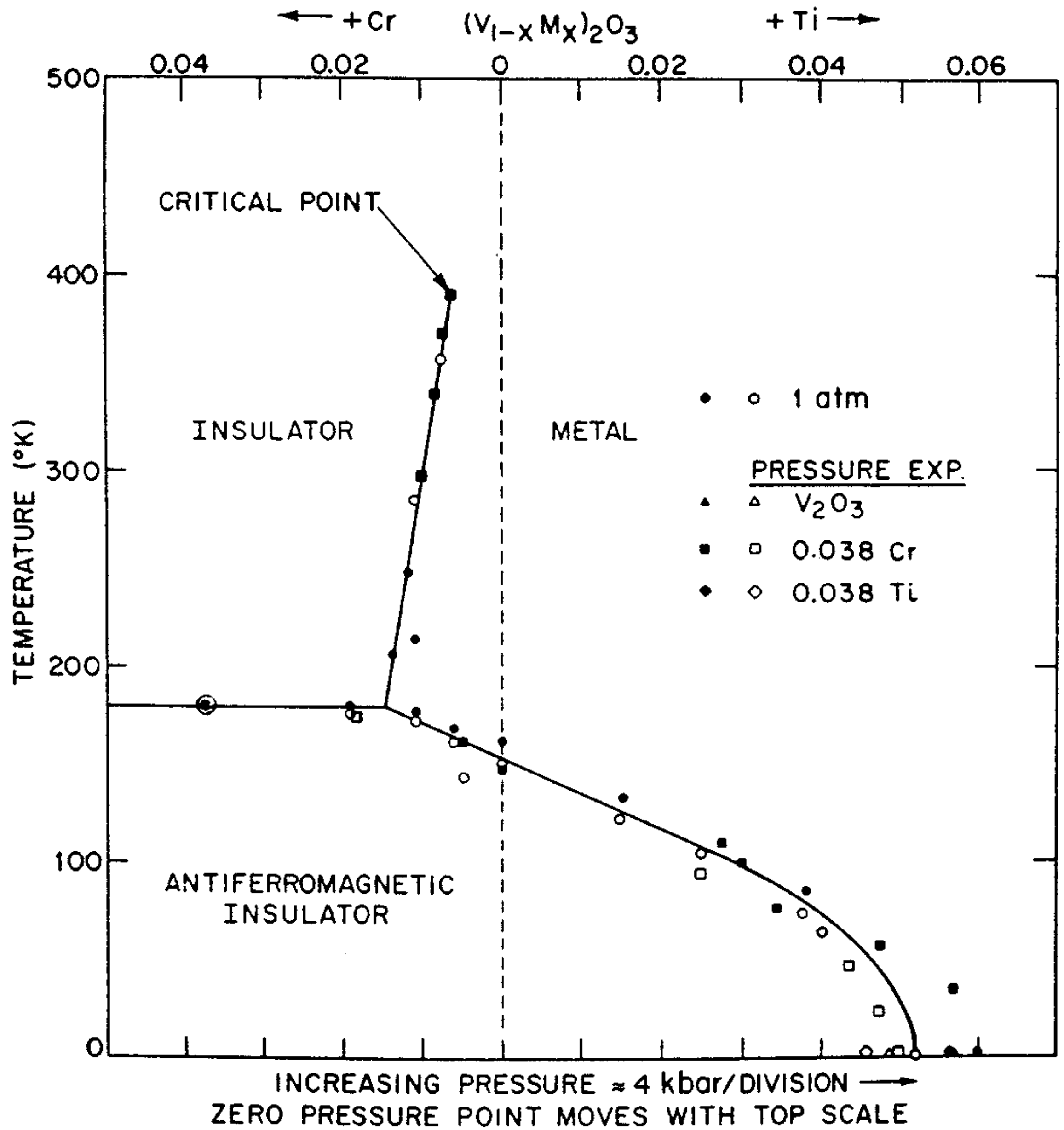
$$\boxed{H = J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \right) \qquad J = \frac{4t^2}{U} > 0}$$

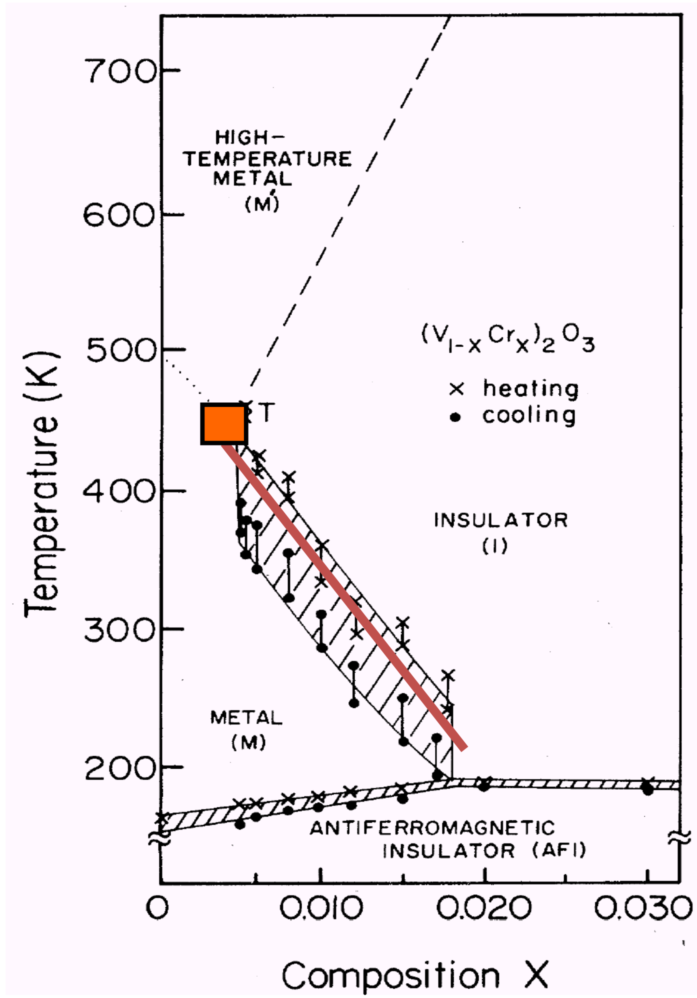
$J>0$: FAVORECE O AFM

$J<0$: " O FM

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

V_2O_3

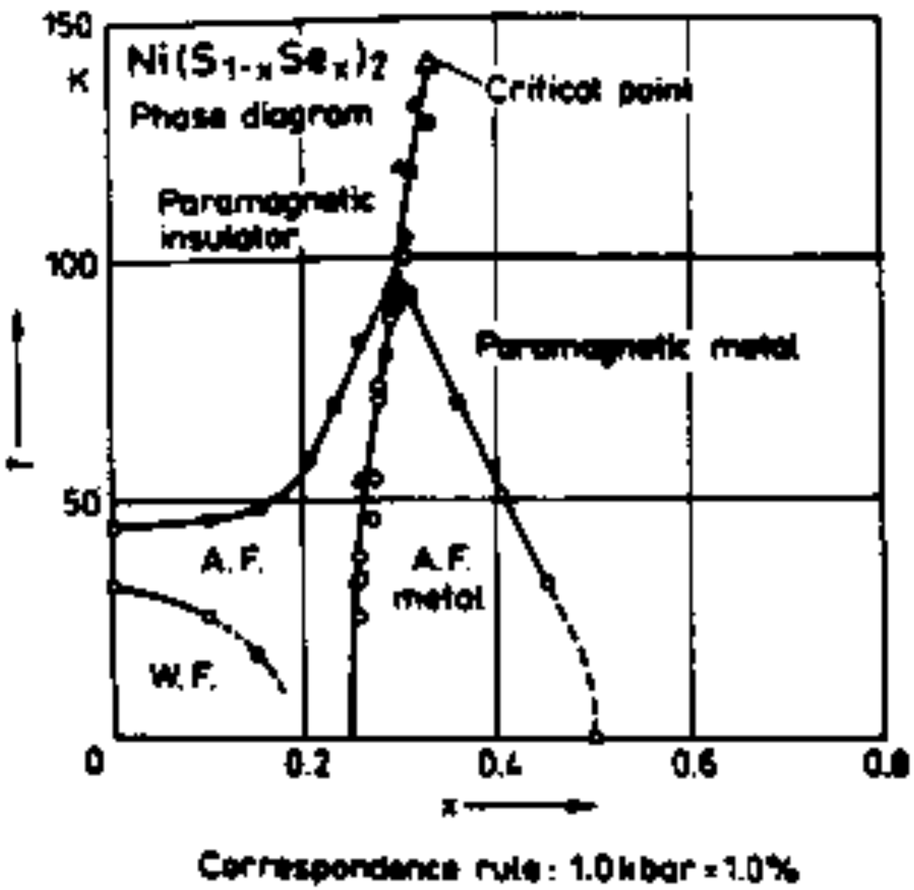




Kuwamoto, PRB '80

- 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.

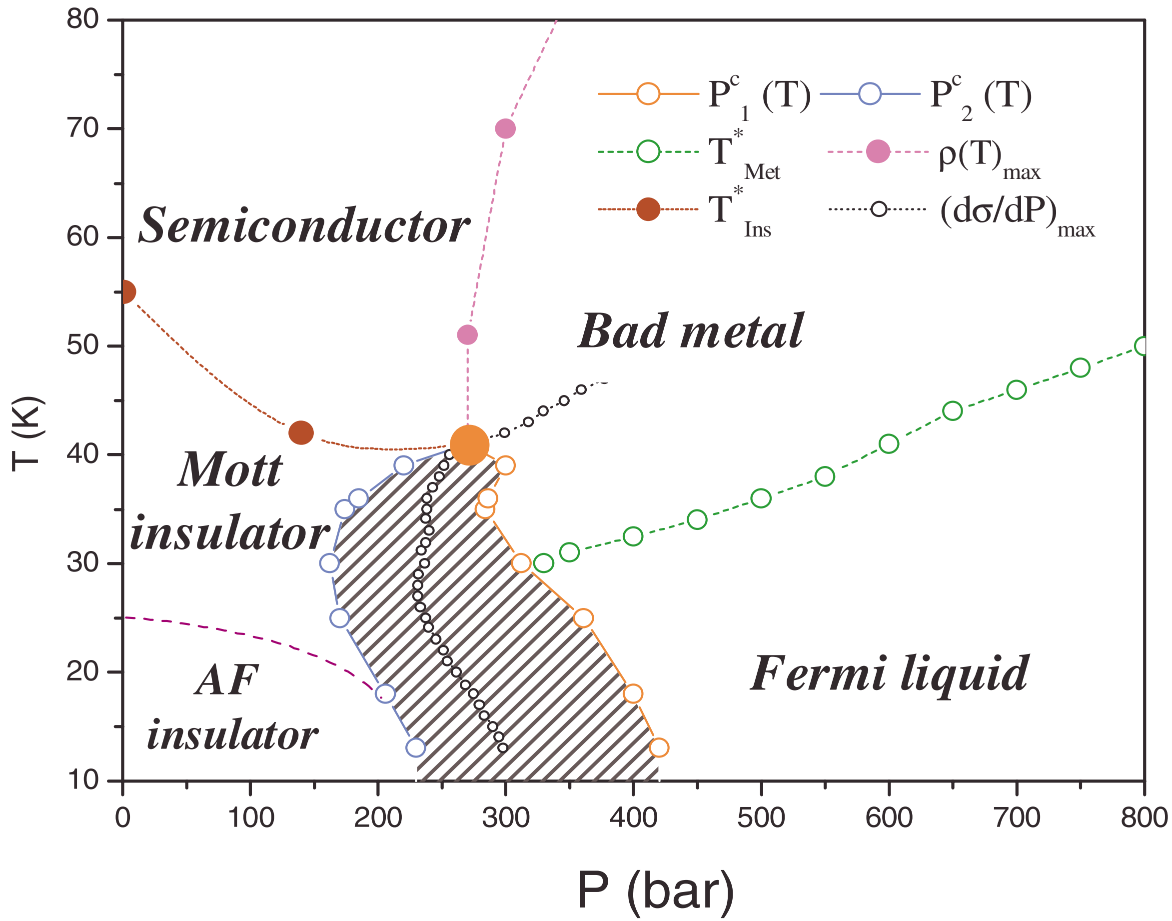
$Ni(S_{1-x}Se_x)_2$



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

Condutores orgânicos fortemente bi-dimensionais

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



Teoria de ondas de spin

$$\boxed{H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j}$$

- CASO $J<0 \Rightarrow$ FM
- BAIXAS TEMPERATURAS, DENTRO DA FASE ORDENADA.
- CONSIDERAR $\underline{S}$ QUALQUER

SIMETRIA: INVARIANTE POR ROTAÇÕES GLOBAIS DOS SPINS. MATEMATICAMENTE:

$$\vec{S}_T = \sum_i \vec{S}_i \Longrightarrow [H, \vec{S}_T] = 0 \quad \text{(PROVEM)}$$

OPERADOR UNITÁRIO DE ROTAÇÕES GLOBAIS:

$$U(\theta, \hat{n}) = \exp\left[i\theta \vec{S}_T \cdot \hat{n}\right] \Rightarrow$$ ROTAÇÃO DE $\underline{\theta}$ EM TORNO DE $\hat{n}$

$$U H U^{-1} = H \Rightarrow [U, H] = 0$$

PODEMOS DIAGONALIZAR $\underline{H}$, $\vec{S}_T^{\,2}$, S_{Tz} SIMULTANEAMENTE: PODEMOS TRABALHAR EM SETORES DE S_{Tz} BEM DEFINIDOS. SE O SISTEMA TEM $\underline{N}$ SÍTIOS:

$S_{Tz} = NS$ (TODOS OS SPINS TEM $M=S$)

$S_{Tz} = (N-1)S + (S-1) = NS - 1$

(TODOS OS SPINS MENOS UM TÊM $M=S$ E O DIFERENTE TEM $M=S-1$)

$S_{Tz} = NS - 2$

$\vdots$

O ESTADO $|\overset{M=S}{\uparrow}\uparrow\uparrow\ldots\rangle$ É AUTO-ESTADO DE $\underline{H}$ E É O ESTADO FUNDAMENTAL

$$\vec{S}_i \cdot \vec{S}_j = \underbrace{\frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)}_{S_{ix}S_{jx} + S_{iy}S_{jy}} + S_{iz} S_{jz}$$

$$\left[\frac{1}{2}\left(S_i^+ S_j^- + h.c.\right) + S_{iz} S_{jz}\right] |\uparrow\uparrow \cdots \uparrow\rangle = S^2 |\uparrow\uparrow\uparrow \ldots\rangle$$

$$S_i^+ |m = s\rangle = 0$$

$$\Rightarrow \left(H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j\right) |\uparrow\uparrow\uparrow \ldots\rangle = -JS^2 \frac{Nz}{2} |\uparrow\uparrow\uparrow \ldots\rangle$$

ONDE z É O NÚMERO DE 1ºS VIZINHOS.

QUALQUER DESVIO DE m_i DE S PARA $S-p$ AUMENTA ESSA ENERGIA:

$$E_0 = -\frac{JNS^2 z}{2}$$

VAMOS CONSIDERAR "UM SPIN FLIP":

$M_i \to S \to S-1$

$$\frac{1}{2}\left[S_i^+ S_j^- + h.c.\right] |\uparrow\downarrow\rangle \qquad (\text{SPIN } S = 1/2)$$

$$= \frac{1}{2} |\downarrow\uparrow\rangle$$

O TERMO S^+S^- TENDE A DELOCALIZAR ESSE ÚNICO SPIN FLIP E OS AUTO-ESTADOS DE $\underline{H}$ SERÃO "ONDAS PLANAS" COM MOMENTO $\vec{k}$:

$$|\vec{k}\rangle = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} |\uparrow\uparrow \ldots, i=\downarrow, \uparrow\uparrow\uparrow\rangle$$

$\Rightarrow$ "ONDA DE SPIN" $\searrow$ SOLUÇÃO EXATA NO SETOR DE 1 S.F.

OS SETORES DE UM NÚMERO FINITO DE SPIN FLIPS NÃO PERMITEM SOLUÇÃO EXATA. SE FOCARMOS NO REGIME EM QUE A DENSIDADE DE SPIN FLIPS É BAIXA PODEMOS TRATAR O SISTEMA COMO UM GÁS FRACAMENTE INTERAGENTE DE "ONDAS DE SPINS"

Transformação de Holstein-Primakoff

MAPEAR ESTADOS E OPERADORES EM UM SISTEMA BOSÔNICO EQUIVALENTE. PARA UM DADO SÍTIO:

ESTADOS: $|S\rangle \longrightarrow |0\rangle$

$|S-1\rangle \longrightarrow |1\rangle$

$|S-2\rangle \longrightarrow |2\rangle$

$\vdots$

$|-S\rangle \longrightarrow |2S\rangle$

$|\delta\rangle \quad \delta = \{0, \dots, 2S\}$

$\boxed{\delta \equiv S - M}$

$|0\rangle$ VÁCUO, $|1\rangle = a^{\dagger}|0\rangle$, $|2\rangle = \frac{(a^{\dagger})^2}{\sqrt{2}}|0\rangle$

$\dots \quad |\delta\rangle = \frac{(a^{\dagger})^{\delta}}{\sqrt{\delta!}}|0\rangle$

OS ESPAÇOS DE HILBERT SÓ SÃO ISOMÓRFICOS SE $\delta = a^{\dagger}a \leq 2S$

OPERADORES:

$$S_z|\mu\rangle = \mu|\mu\rangle$$

$$\Downarrow$$

$$S_z|\delta\rangle = (S-\delta)|\delta\rangle$$

$$= (S - a^{\dagger}a)|\delta\rangle$$

$$\boxed{S_z \longleftrightarrow S - a^{\dagger}a}$$

$$S^{\pm}|\mu\rangle = \sqrt{(S\mp\mu)(S\pm\mu+1)}\,|\mu\pm1\rangle$$

$$S^{\pm}|\delta\rangle = \left\{\left[S\mp(S-\delta)\right]\left[S+1\pm(S-\delta)\right]\right\}^{1/2}|\delta\mp1\rangle$$

$$S^{+}|\delta\rangle = \left\{[\delta][2S+1-\delta]\right\}^{1/2}|\delta-1\rangle$$

$$S^{+}|\delta\rangle = \sqrt{2S}\sqrt{1-\frac{(\delta-1)}{2S}}\sqrt{\delta}\,|\delta-1\rangle$$

$$\boxed{S^{+} \longleftrightarrow \sqrt{2S}\sqrt{1-\frac{a^{\dagger}a}{2S}}\;a\;;\quad S^{-} \longleftrightarrow \sqrt{2S}\,a^{\dagger}\sqrt{1-\frac{a^{\dagger}a}{2S}}}$$

MAIS RIGOROSAMENTE, PROVEM QUE AS ASSOCIAÇÕES ACIMA SATISFAZEM A ÁLGEBRA DE SPIN.

PARA UMA REDE DE SPINS: $a, a^+ \rightarrow a_i, a_i^+$

LEVANDO EM H:

TRANSFORMAÇÃO DE HOLSTEIN-PRIMAKOFF:

$$S_{iz} \rightarrow S - a_i^+ a_i$$

$$S_i^+ \rightarrow \sqrt{2S}\sqrt{1 - \frac{a_i^+ a_i}{2S}}\, a_i$$

$$S_i^- \rightarrow \sqrt{2S}\, a_i^+ \sqrt{1 - \frac{a_i^+ a_i}{2S}}$$

$$\sum_{\langle ij \rangle} S_{iz} S_{jz} = \sum_{\langle ij \rangle} (S - \hat{n}_i)(S - \hat{n}_j) = \frac{Nz}{2} S^2 - S\left[\sum_{\langle ij \rangle} (\hat{n}_i + \hat{n}_j)\right]$$

$$+ \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j = \frac{NS^2 z}{2} - Sz \sum_i \hat{n}_i + \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$

NOTEM A ORDEM DECRESCENTE EM S O QUE SUGERE UMA EXPANSÃO SEMI-CLÁSSICA EM $\left(\frac{1}{S}\right)$.

$$\frac{1}{2}\sum_{\langle ij\rangle}\left(S_i^+ S_j^- + h.c.\right) = \frac{1}{2}\sum_{\langle ij\rangle}\left[(2S)\left[1-\frac{\hat{n}_i}{2S}\right]^{1/2} a_i\, a_j^\dagger \left[1-\frac{\hat{n}_j}{2S}\right]^{1/2} + h.c.\right]$$

APROXIMAÇÕES NO REGIME: $\langle n_i \rangle \ll 2S$ E/OU $\frac{1}{S} \ll 1$

$$H \cong \overbrace{-\frac{JNS^2 z}{2}}^{E^0} + JSz\sum_i \hat{n}_i - JS\sum_{\langle ij\rangle}\left(a_i a_j^\dagger + h.c.\right) + O(S^0)$$

$$= E^0 + JSz\sum_i \hat{n}_i - JS\sum_{\langle ij\rangle}\left(a_i^\dagger a_j + h.c.\right) + O(S^0)$$

SOLUÇÃO POR TRANSF. DE FOURIER:

$$a_k^\dagger = \frac{1}{\sqrt{N}}\sum_i e^{i\vec{k}\cdot\vec{R}_i}\, a_i^\dagger, \ldots$$

$$H = E_0 + JSz \sum_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}} - JS \sum_{\vec{k}} \gamma_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}}$$

$$\gamma_{\vec{k}} = \left(\sum_{\langle oj \rangle} e^{i \vec{k} \cdot \vec{R}_j} + c.c. \right) = 2 \left(\cos k_x + \cos k_y + \cos k_z \right)$$

$(a = 1)$

$$\boxed{H = E_0 + \sum_{\vec{k}} \epsilon_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}}}$$

$$\epsilon_{\vec{k}} = JSz \left[1 - \frac{1}{z} \gamma_{\vec{k}} \right] = JSz \left[1 - \frac{\cancel{2}}{\cancel{2}D} \left(\cos k_1 \cdots \cos k_D \right) \right]$$

SE $k \ll 1$:
$$\epsilon_{\vec{k}} = JS \left[k_1^2 + k_2^2 + \cdots k_D^2 \right]$$

$$= JS |\vec{k}|^2$$

A DISPERSÃO DOS "MAGNONS" FM É QUADRÁTICA PARA k PEQUENO.

Sistema em equilíbrio à temperatura T

$$\langle \hat{n}_{\vec{k}} \rangle = \langle a^\dagger_{\vec{k}} a_{\vec{k}} \rangle = \frac{1}{e^{\beta \epsilon_{\vec{k}}} - 1} = b(\epsilon_{\vec{k}}) \quad (\text{PLANCK})$$

BÓSONS COM POTENCIAL QUÍMICO $\mu = 0$. SEU NÚMERO MÉDIO É DETERMINADO APENAS PELA TEMPERATURA.

$$U(T) = E_0 + \sum_{\vec{k}} \epsilon_{\vec{k}} \langle \hat{n}_{\vec{k}} \rangle = E_0 + V \int \frac{d^D k}{(2\pi)^D} \frac{\epsilon_{\vec{k}}}{e^{\beta \epsilon_{\vec{k}}} - 1}$$

SE $T \ll J$:

$$\Delta U(T) = V \int \frac{d^D k}{(2\pi)^D} \frac{JSk^2}{e^{\beta J S k^2} - 1} \qquad \vec{x} = \sqrt{\beta J S}\, \vec{k}$$

EM 3D: $\Delta U(T) \propto \int d^3x \frac{x^2}{e^{x^2} - 1} (\beta J S)^{-5/2} \propto T^{5/2}$

$$C(T) = \frac{\partial \Delta U}{\partial T} \propto T^{3/2}$$

MAGNETIZAÇÃO: $M_z = g\mu_B \sum_i \langle m_i \rangle$

$$= g\mu_B \sum_i \left[S - \langle a_i^\dagger a_i \rangle \right]$$

$$= g\mu_B N S - g\mu_B \sum_{\vec{k}} \langle \hat{n}_{\vec{k}} \rangle$$

$$\Delta M(T) = -M_z(T) + M_z(0) = g\mu_B \sum_{\vec{k}} \langle \hat{n}_{k} \rangle$$

$$= g\mu_B V \int \frac{d^D k}{(2\pi)^D} \frac{1}{e^{\beta \epsilon_{\vec{k}}} - 1}$$

$T \ll J$ (3D):

$$\Delta M(T) \propto \int d^3x \, \frac{1}{e^{x^2} - 1} (\beta J S)^{-3/2} \propto T^{3/2}$$

PARA D GENÉRICO: $T \ll J$

$$\Delta M(T) \propto \int d^D k \, \frac{1}{e^{\beta J S k^2} - 1} \underset{T \ll J}{\sim} \int_0^{\Lambda} \frac{k^{(D-1)} \, dk}{k^2}$$

$$\sim \int_0^{\Lambda} k^{(D-3)} \, dk$$

$D \leq 2$: A INTEGRAL DIVERGE EM $k \to 0$

ESSA DIVERGÊNCIA SUGERE QUE A CORREÇÃO À MAGNETIZAÇÃO DIVERGE EM $D \leq 2$ COMO VIMOS NO CASO DOS BOGOLIUBONS.

TEOREMA RIGOROSO DE "MERMIN-WAGNER"

Dispersão de magnons num FM

PRL **108,** 197205 (2012) PHYSICAL REVIEW LETTERS week ending 11 MAY 2012

Magnon Lifetimes on the Fe(110) Surface: The Role of Spin-Orbit Coupling

Kh. Zakeri,* Y. Zhang, T.-H. Chuang, and J. Kirschner
Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany
(Received 16 January 2012; published 9 May 2012)

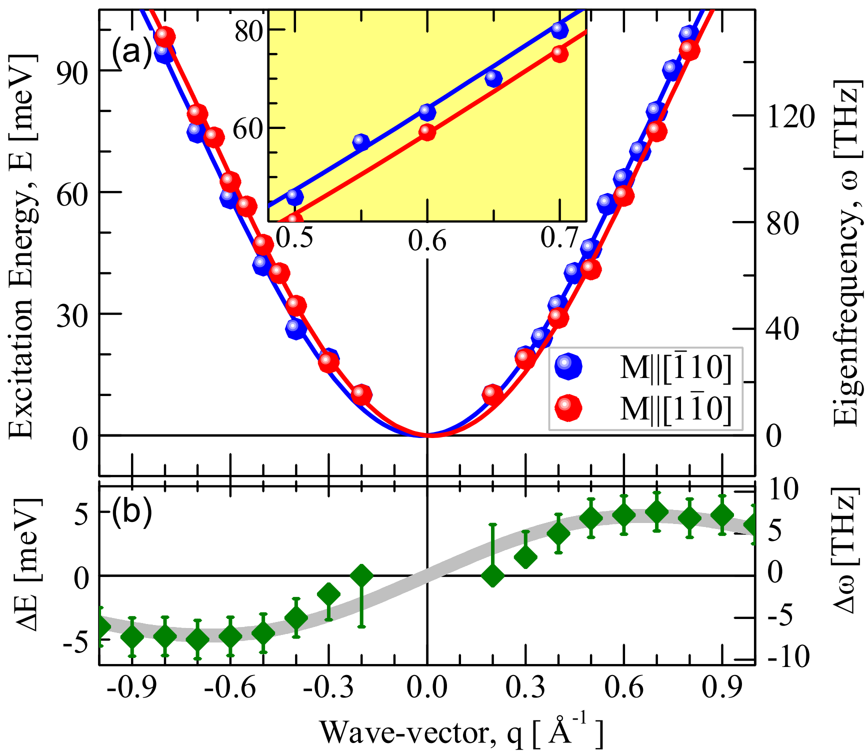


FIG. 1 (color online). (a) Magnon dispersion relation measured on a 2 ML Fe on W(110) at room temperature and for two different magnetization directions. The inset shows a magnified part of the graph for a smaller energy and wave-vector window. (b) The energy splitting defined as $\Delta E(q) = E_{M\|[\bar{1}10]}(q) - E_{M\|[1\bar{1}0]}(q)$ obtained from (a). The symbols represent the experimental results, while the solid lines represent the fits based on the extended Heisenberg spin Hamiltonian.

Dispersão de magnons num FM

Magnon spectrum and related finite-temperature magnetic properties: A first-principle approach
S. V. Halilov, A. Y. Perlovgif, P. M. Oppeneer and H. Eschrig
Europhys. Lett, **39**, 91-96 (1997)

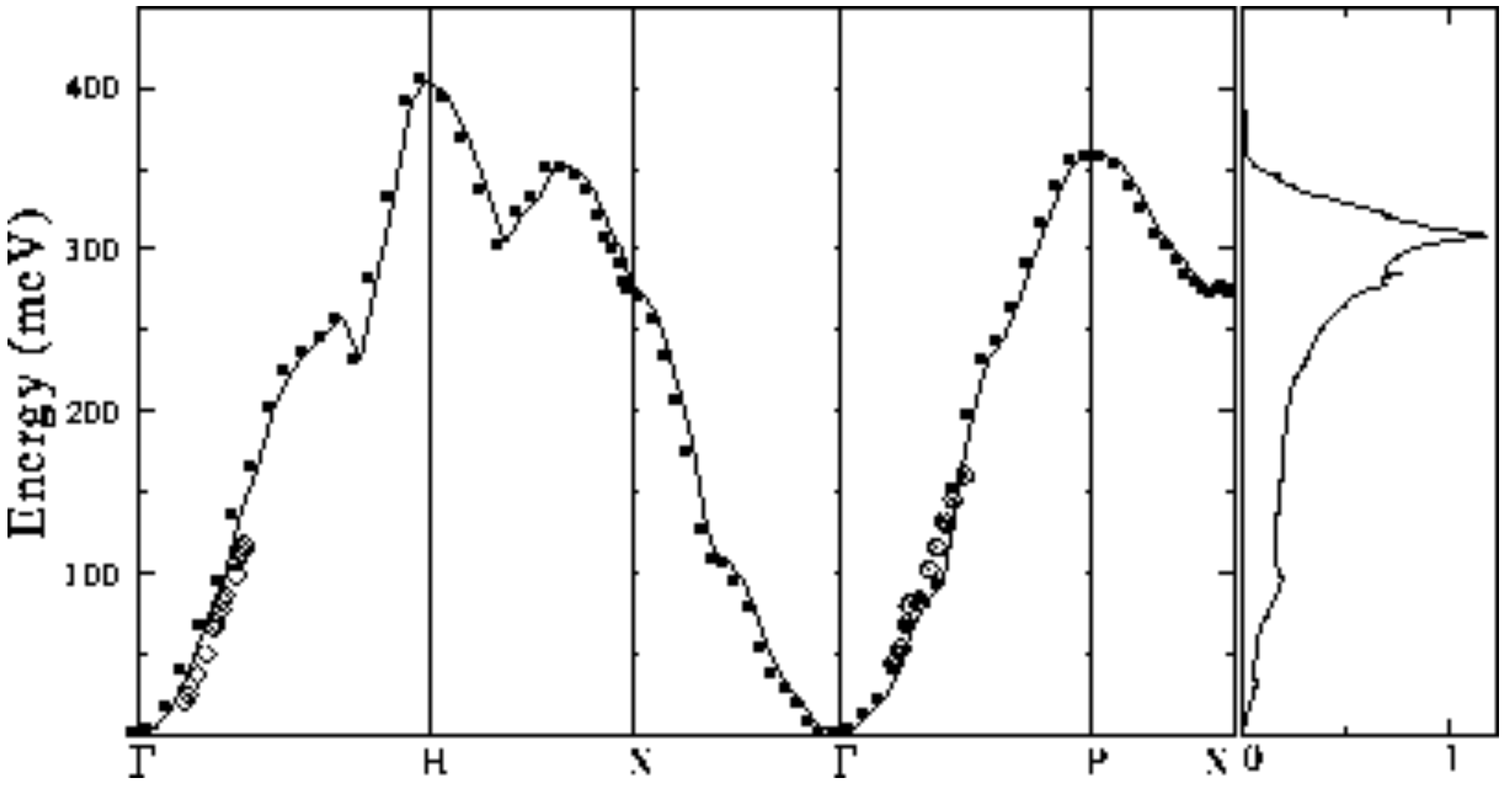
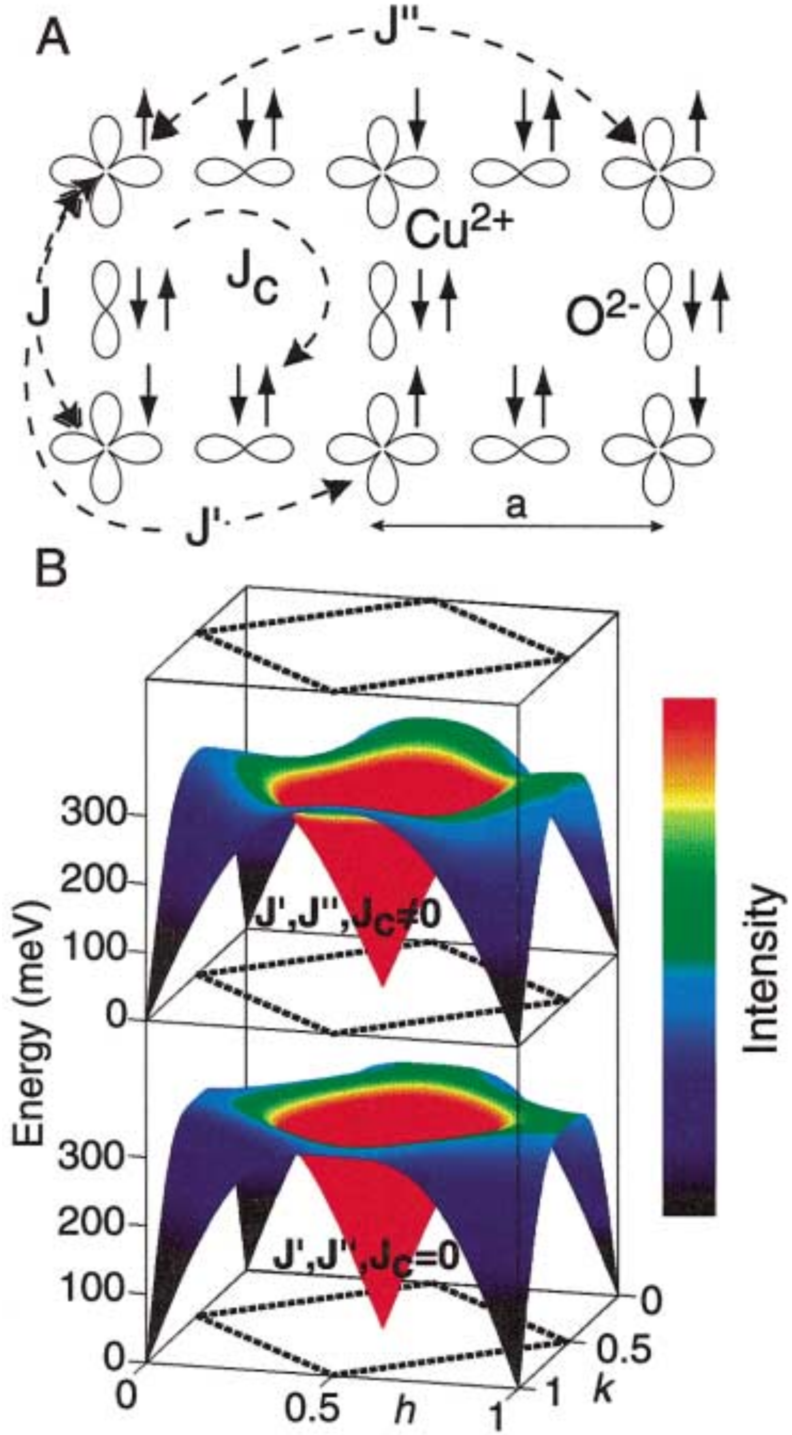


Figure 1: Magnon dispersions of bcc Fe for high-symmetry directions. Experimental data, for pure Fe at 10 K: [20], and for Fe (12 Si) at room temperature: [22]. Calculated dispersions are depicted by solid circles and line. The right-hand panel shows the calculated magnon total density of states (in states/(meVcell)). Note the Kohn-like anomalies ("cusps'') in the theoretical spectrum.

Magnons em um AFM

Spin waves and electronic interactions in La_2CuO_4, R. Coldea *et al.*, Phys. Rev. Lett. **86**, 5377 (2001)



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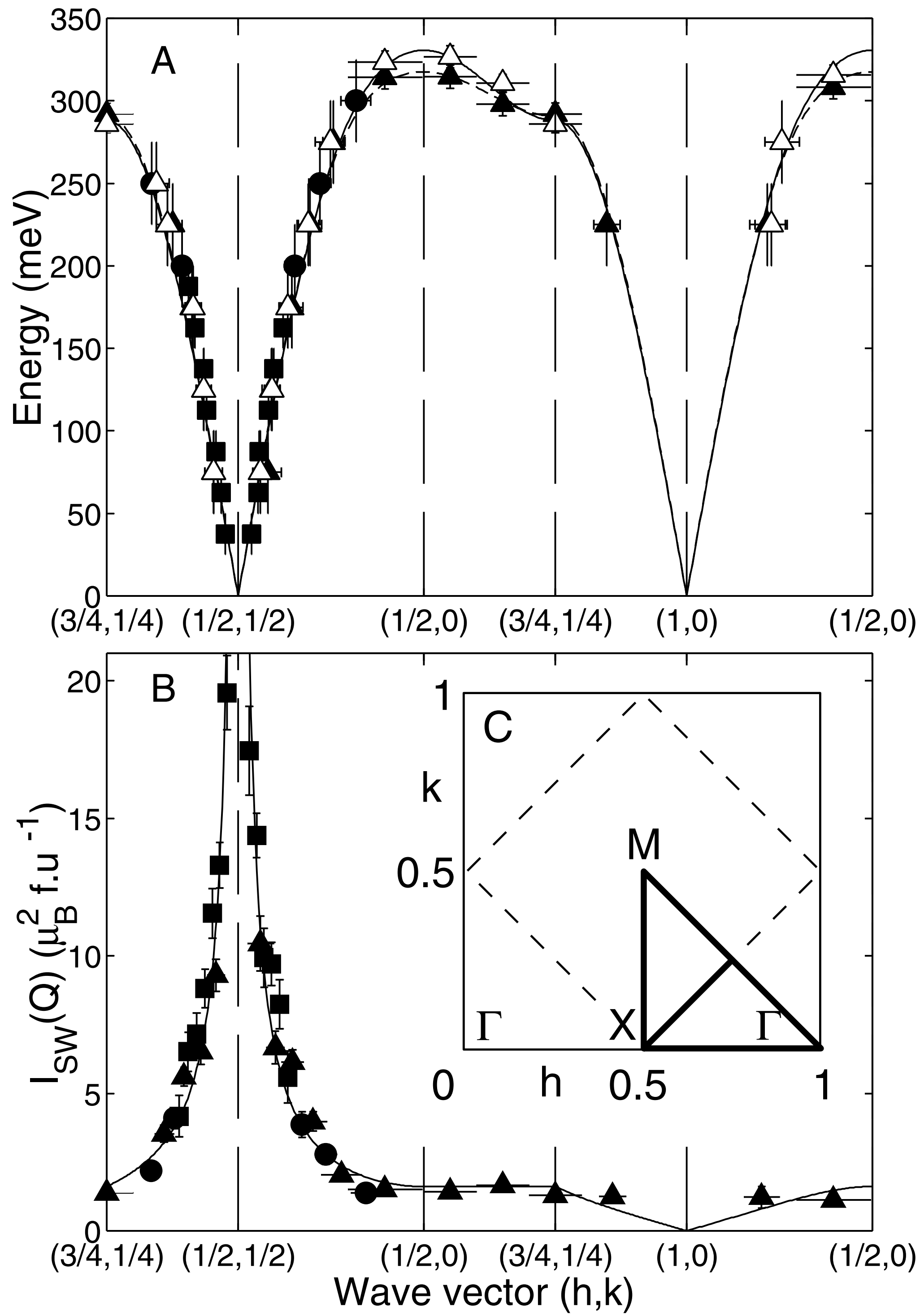
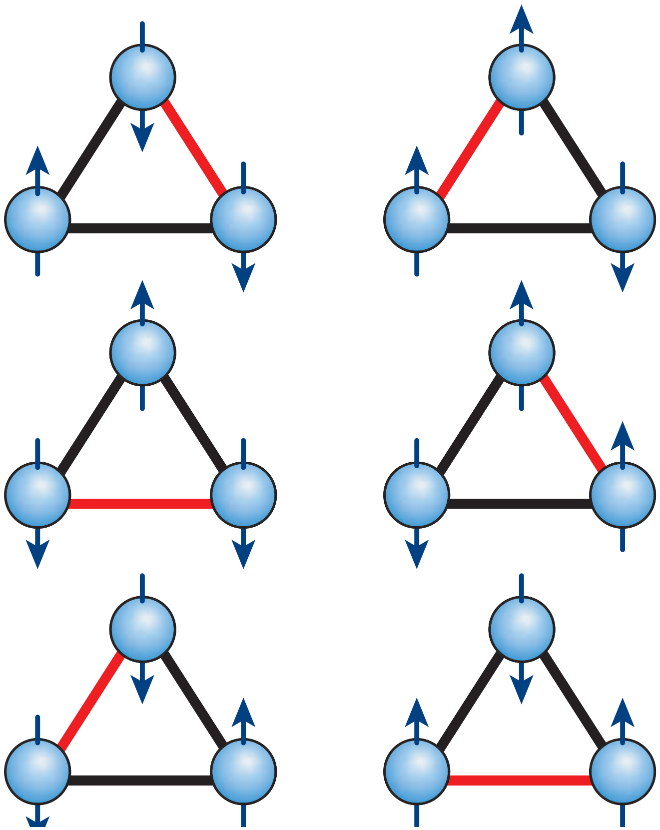


Frustração



Frustração

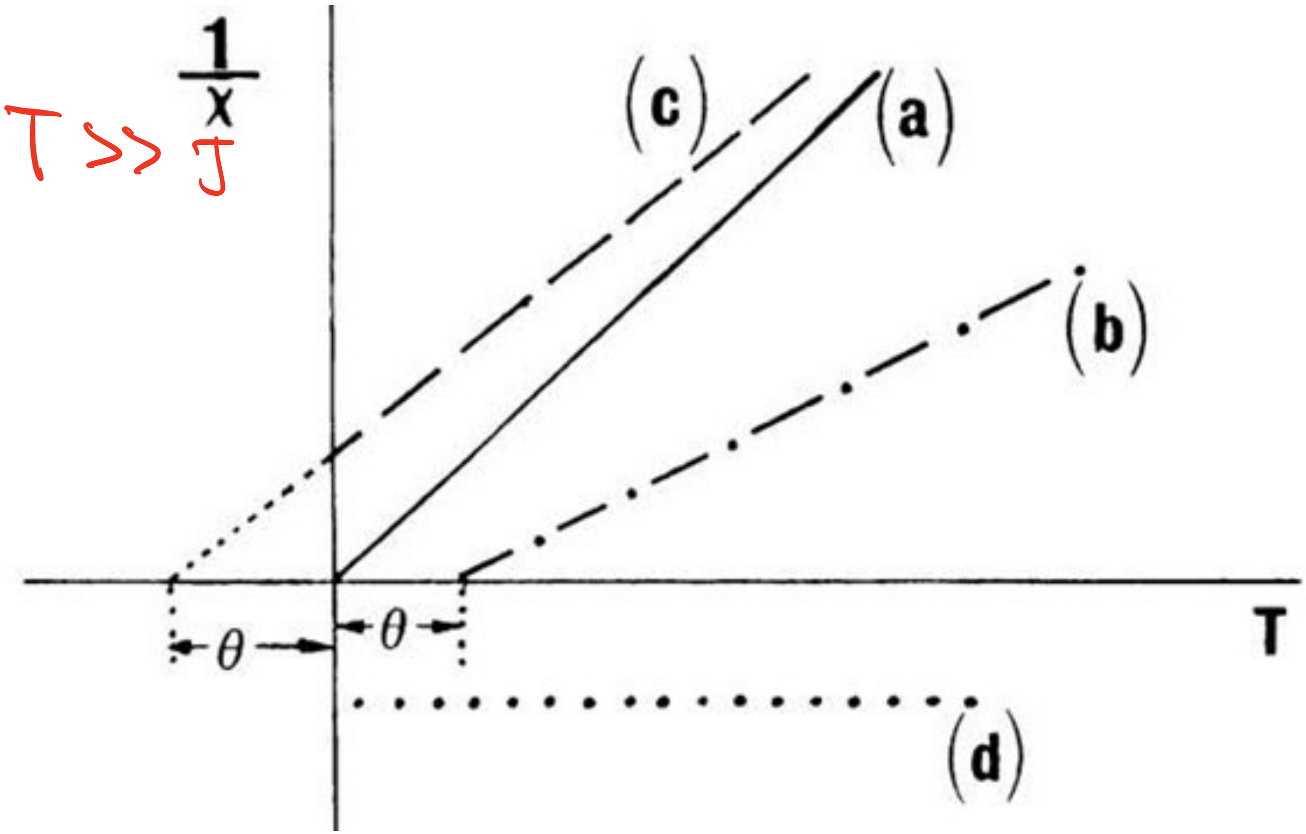
Lei de Curie-Weiss

$$\chi = \frac{1}{T - \theta} \qquad T \gg J$$

$\theta \propto (-J)$

$\theta > 0$ FM

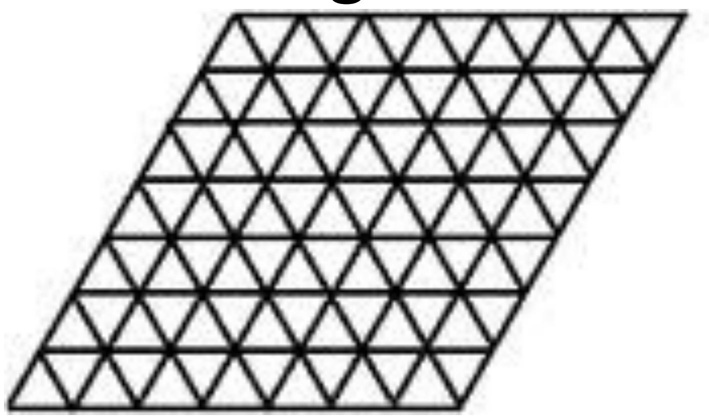
$\theta < 0$ AFM



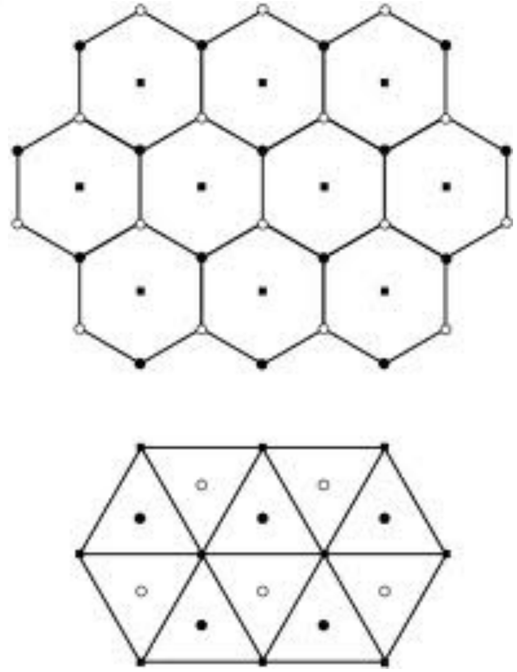
MEDIDA DE FRUSTRAÇÃO: $\frac{\theta}{T_N}$

Algumas redes frustradas

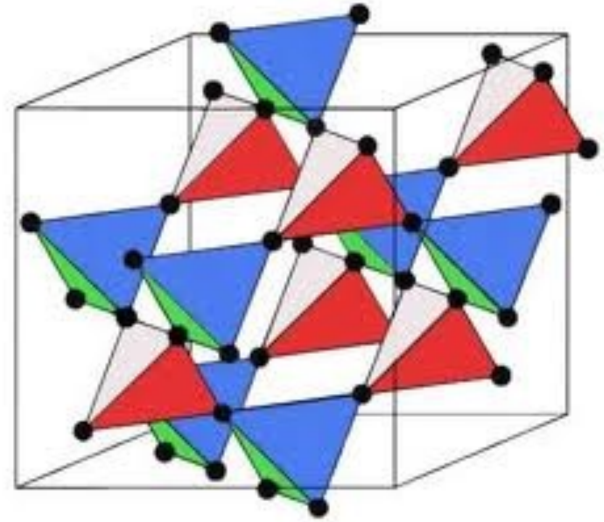
Triangular



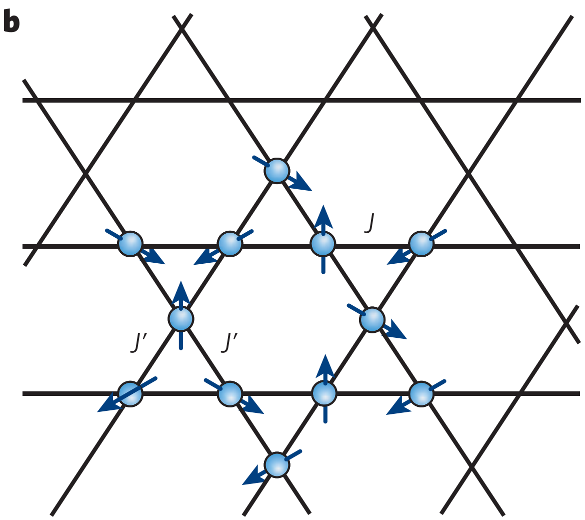
Hexagonal



Pirocloro



Kagomé



Frustração

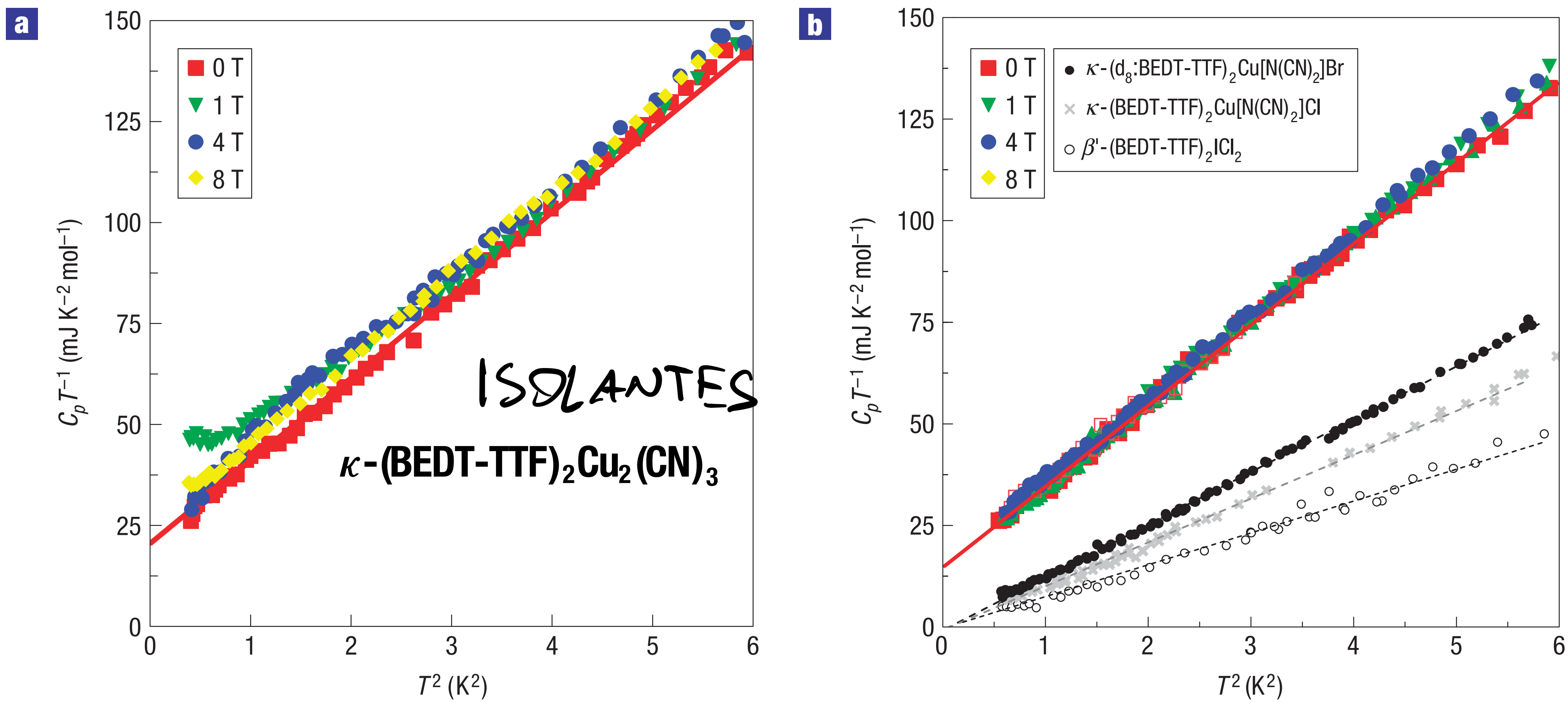
Table 1 | Some experimental materials studied in the search for QSLs

Material	Lattice	S	Θ_{CW} (K)	R*	Status or explanation
κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$	Triangular†	½	−375‡	1.8	Possible QSL
EtMe$_3$Sb[Pd(dmit)$_2$]$_2$	Triangular†	½	−(375–325)‡	?	Possible QSL
Cu$_3$V$_2$O$_7$(OH)$_2$•2H$_2$O (volborthite)	Kagomé†	½	−115	6	Magnetic
ZnCu$_3$(OH)$_6$Cl$_2$ (herbertsmithite)	Kagomé	½	−241	?	Possible QSL
BaCu$_3$V$_2$O$_8$(OH)$_2$ (vesignieite)	Kagomé†	½	−77	4	Possible QSL
Na$_4$Ir$_3$O$_8$	Hyperkagomé	½	−650	70	Possible QSL
Cs$_2$CuCl$_4$	Triangular†	½	−4	0	Dimensional reduction
FeSc$_2$S$_4$	Diamond	2	−45	230	Quantum criticality

BEDT-TTF, bis(ethylenedithio)-tetrathiafulvalene; dmit, 1,3-dithiole-2-thione-4,5-ditholate; Et, ethyl; Me, methyl. *R is the Wilson ratio, which is defined in equation (1) in the main text. For EtMe$_3$Sb[Pd(dmit)$_2$]$_2$ and ZnCu$_3$(OH)$_6$Cl$_2$, experimental data for the intrinsic low-temperature specific heat are not available, hence R is not determined. †Some degree of spatial anisotropy is present, implying that $J' \neq J$ in Fig. 1a. ‡A theoretical Curie–Weiss temperature (Θ_{CW}) calculated from the high-temperature expansion for an S = ½ triangular lattice; $\Theta_{CW} = 3J/2k_B$, using the J fitted to experiment.

L. Balents, Nature **464**, 199 (2010)

Calor específico linear em T



S. Yamashita *et al.*, Nature Phys. **4**, 459 (2008)

Calor específico linear em T é típico de férmions. Em algumas teorias, as excitações elementares são férmions neutros (“spinons”)

Condutividade térmica linear em T?

Essas mesmas excitações fermiônicas neutras ("spinons") deveriam dar origem a $\kappa(T) \sim T$.

Mas o resultado experimental é exponencial (gap?)

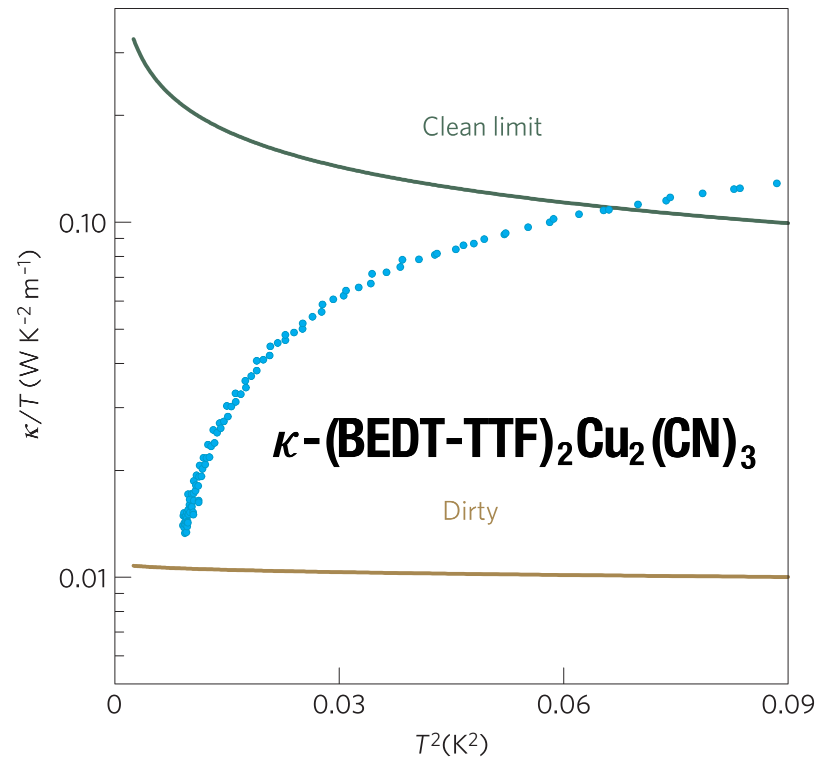


Figure 3 | Comparison between the data and the theory based on the gapless QSL with a spinon Fermi surface. κ/T data (sample A) in zero field (blue) plotted together with expected dependence of equation (1). The green line is for the clean limit ($1/\tau = 0$) and brown for a dirty case with the mean free path as short as $10a$, where $a(\simeq 0.8$ nm) is the lattice parameter of the triangular lattice.

M. Yamashita *et al.*, Nature Phys. **5**, 44 (2009)