

TRANSICIONES de FASE CUÁNTICAS

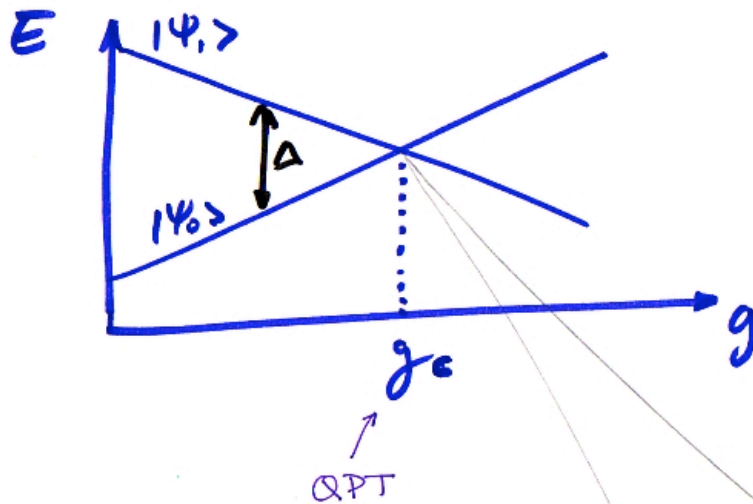
TRANSICIONES a $T=0$
 DEBIDAS A LA VARIACIÓN DE UN PARAMETRO (H, P, x, ...)
NO-TÉRMICO

Ph.Tr. (Classical)

- Papel esencial en la NATURALEZA
- "Cualquier" sistema físico tiene Ph.Tr. (U, H₂O...)
"termodinámico"
- Ocurren como variaciones de un parámetro de control
- $T \neq 0$: ORDEN MACROSCÓPICO vs. FLUCTUACIONES TÉRMICAS
- $T = 0$: SÓLO \exists FLUCTUACIONES CUÁNTICAS

$$\mathcal{H} = \mathcal{H}_0 + g \mathcal{H}_1$$

g : parámetro de control
(H, P, E, x, \dots)



$$\mathcal{H}|\psi_i\rangle = E_i|\psi_i\rangle$$

$$\Delta \sim J|g - g_c|^{2\nu}$$

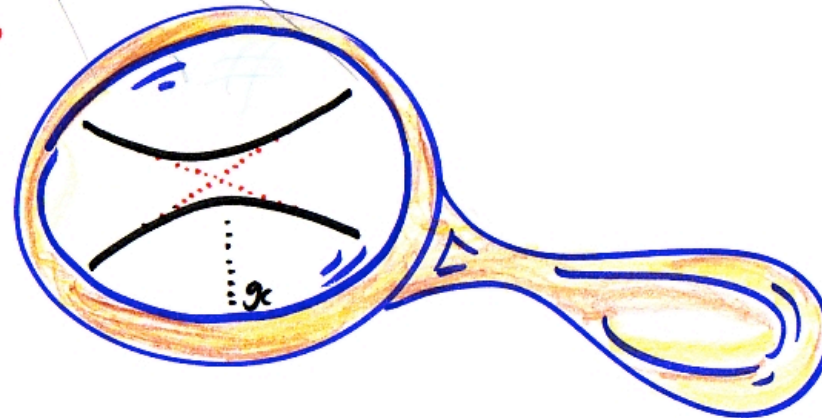
Escala de Energías

0 en QPT

exponente crítico

"Avoided level crossing"

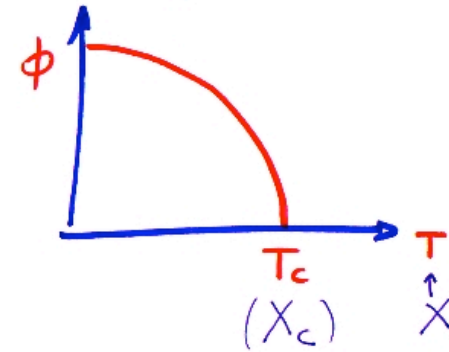
LA QPT VIENE ACOMPAÑADA DE UN CAMBIO CUALITATIVO EN LAS CORRELACIONES DEL ESTADO FUNDAMENTAL



TRANSICIONES CONTINUAS

Order parameter

- $T > T_c \Rightarrow \langle \phi \rangle_T = 0$
pero las fluctuaciones $\delta\phi \neq 0$, en geral.
- CERCA de T_c la LONGITUD de CORRELACIÓN ξ
(l. característica de las $\delta\phi$) DIVERGE:



$$\xi \propto |t|^{-\nu} \quad t = \frac{|T - T_c|}{T_c}$$

- \exists un TIEMPO DE CORRELACIÓN (τ_c) \sim tiempo típico de relajación.

$$\tau_c \propto \xi^z \propto |t|^{-\nu z}$$

$z \equiv$ exponente crítico dinámico

Q.M. cerca del punto crítico.

2 aspectos

QM puede ser fundamental para entender la existencia de la fase ordenada (o ambas); e.g.:

- SUPERCONDUCTIVIDAD
- SUPERFLUIDEZ
- ...

¿Es la Q.M. relevante en el comportamiento crítico (asintótico)?

$$\tau_c \sim |t|^{-\nu z}$$

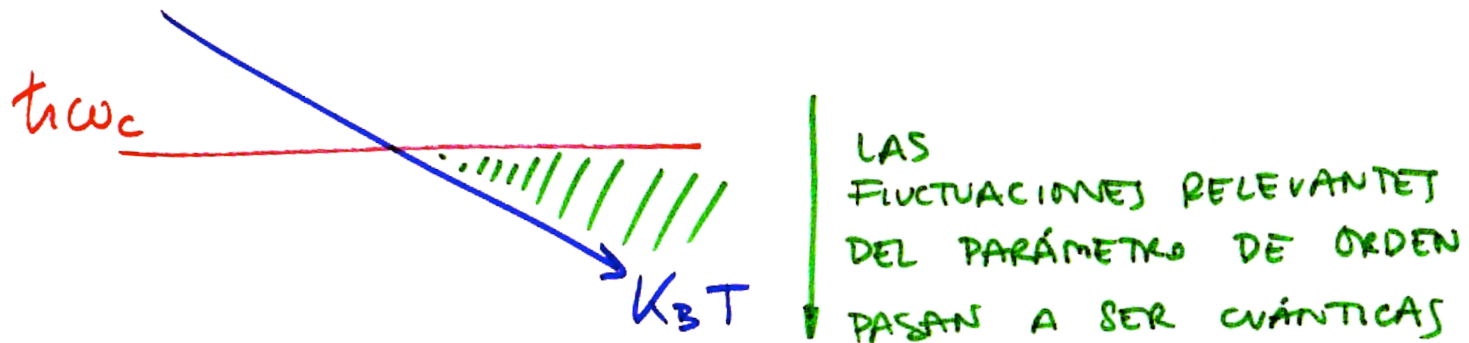
↓

$$h\nu_c \rightarrow k_B T$$

$$h\nu_c \sim |t|^{\nu z}$$

$$\hbar\omega_c \gg k_B T \longrightarrow \text{QM relevante}$$

$$\hbar\omega_c \ll k_B T \longrightarrow \text{Classical description.}$$



pero

$$|t| = \frac{|T - T_c|}{T_c} < T_c^{-1/2}$$

$$\text{y } \hbar\omega_c \sim |t|^{\nu z}$$

suficientemente CERCA de T_c ; $\boxed{\hbar\omega_c \ll k_B T}$ si T_c es finito

$\forall T_c \neq 0 \Rightarrow \text{Ph.Tr. CLÁSICAS}$

• Si T_c es finita ...

- ① LAS FLUCTUACIONES CLÁSICAS DOMINAN LA TRANSICIÓN DE FASE, AUNQUE "SUFICIENTEMENTE CERCA" de T_c PUEDE QUERER DECIR "MUY CERCA!!" SI T_c ES MUY BAJA O LA DINÁMICA LO REQUIERE ...
DA IGUAL: "ASINTÓTICAMENTE", LA TR. ES CLÁSICA
- ② SI $T_c = 0$ \nrightarrow FLUCTUACIONES CLÁSICAS \Rightarrow Q. P. T.
- ③ EL PARÁMETRO DE CONTROL DEL ORDEN ES "NO-TÉRMICO"
- ④ DEPENDIENDO DE SI \exists ORDEN A $T \neq 0$ O NO \rightarrow 2 DIAGRAMAS de FASE

1D = CADENA ISING

2D - XY \rightarrow Kosterlitz-Thouless

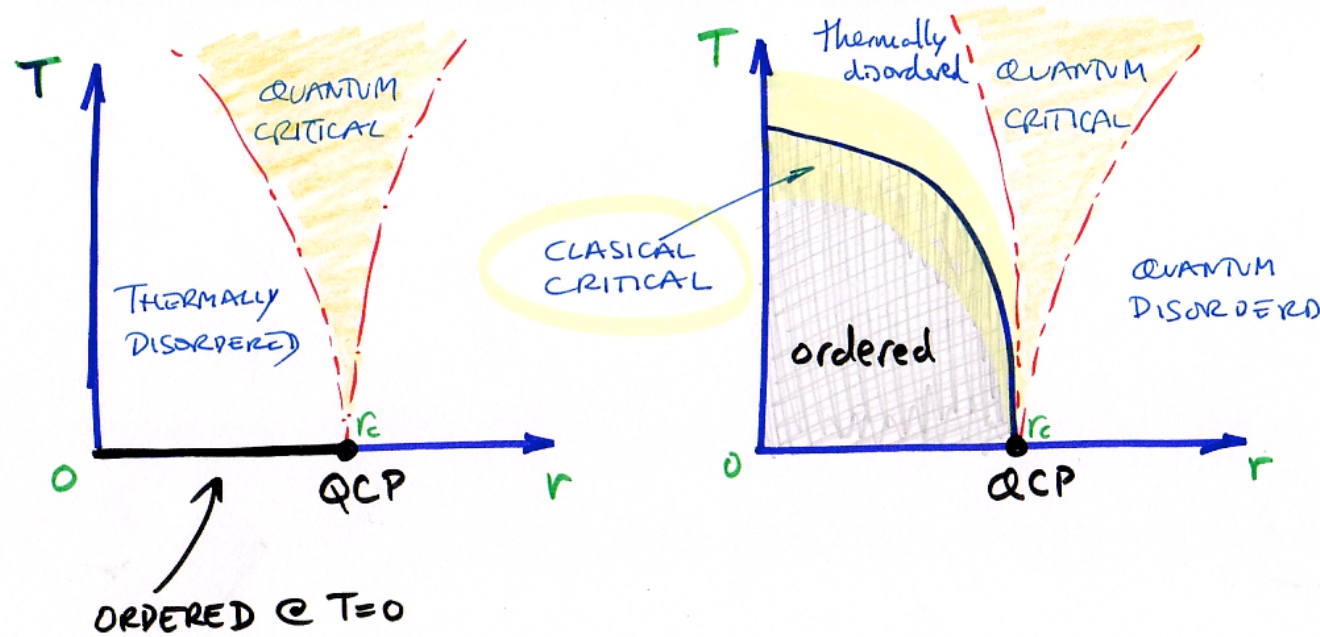
ISING - 2D

FERROMAGNETO REAL

DOPED La_2CuO_4

⋮


④ DEPENDIENDO DE SI \exists ORDEN A $T \neq 0$ O NO \rightarrow 2 DIAGRAMAS de FASE



¿QUÉ HAY EN LA REGIÓN CRÍTICA CUÁNTICA?

- LA FÍSICA ESTA CONTROLADA POR LAS EXCITACIONES TÉRMICAS DEL ESTADO FUNDAMENTAL CUÁNTICO (Las excitaciones no son las habituales, las "leyes de potencias" no son las habituales, Comportamiento de líquido no-de-Fermi ...)

PARÁMETROS NO-TERMICOS EN Q.P.T.

- x ≡ "Composición" $\text{CeCu}_{6-x}\text{Au}_x$
- P ≡ PRESIÓN 
- H ≡ CAMPO MAGNÉTICO

Ejemplo "típico": LiHoF_4 ($T_c = 1.53 \text{ K} @ H = 0$) model system
Ising under field

$$\mathcal{H} = \sum_{\langle i,j \rangle}^N J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_i^N \sigma_i^x$$

σ ≡ Pauli matrices
 J_{ij} ≡ exchange etc.
 Γ ≡ transversal field

Quantum Critical Behavior for a Model Magnet

D. Bitko and T. F. Rosenbaum

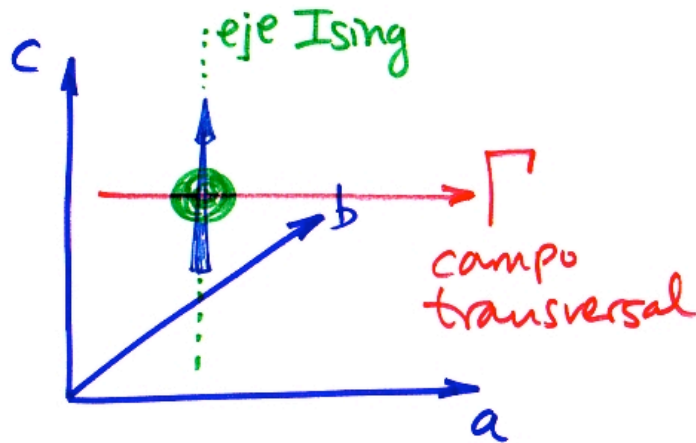
The James Franck Institute and Department of Physics, The University of Chicago, Chicago, Illinois 60637

G. Aeppli

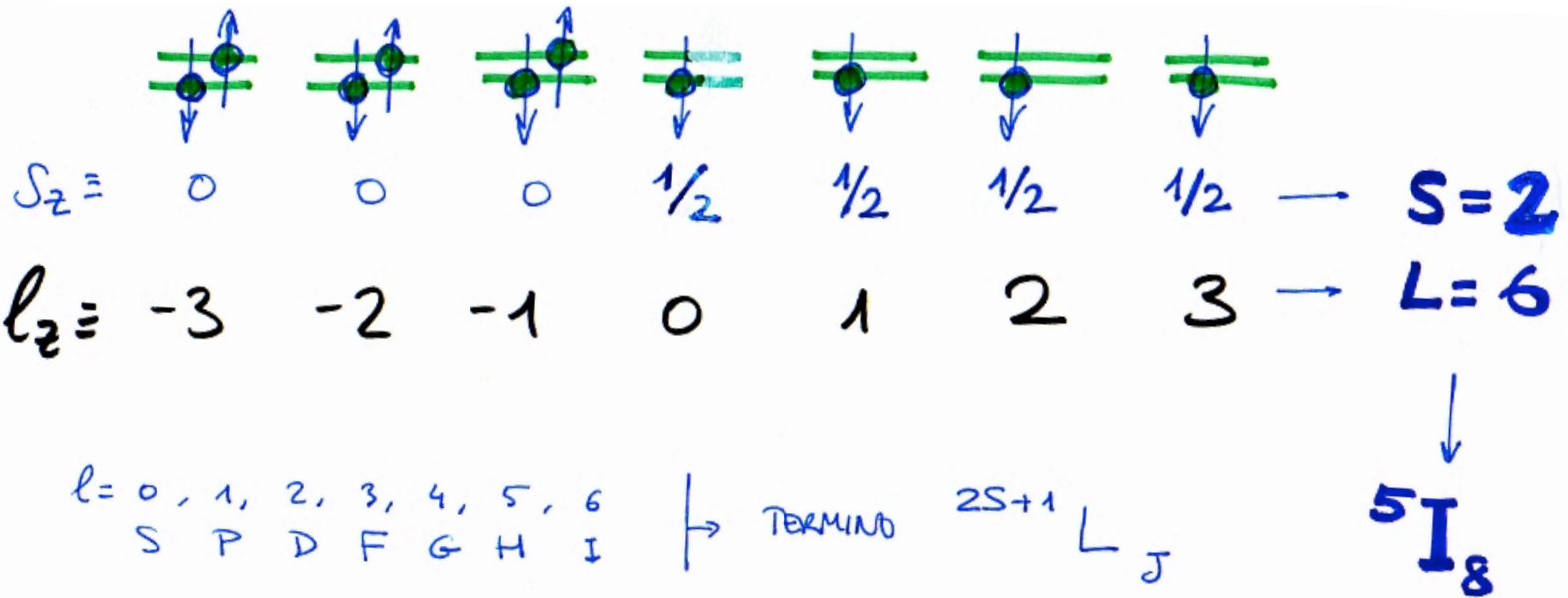
NEC Research Institute, 4 Independence Way, Princeton, New Jersey 08540

(Received 18 March 1996)

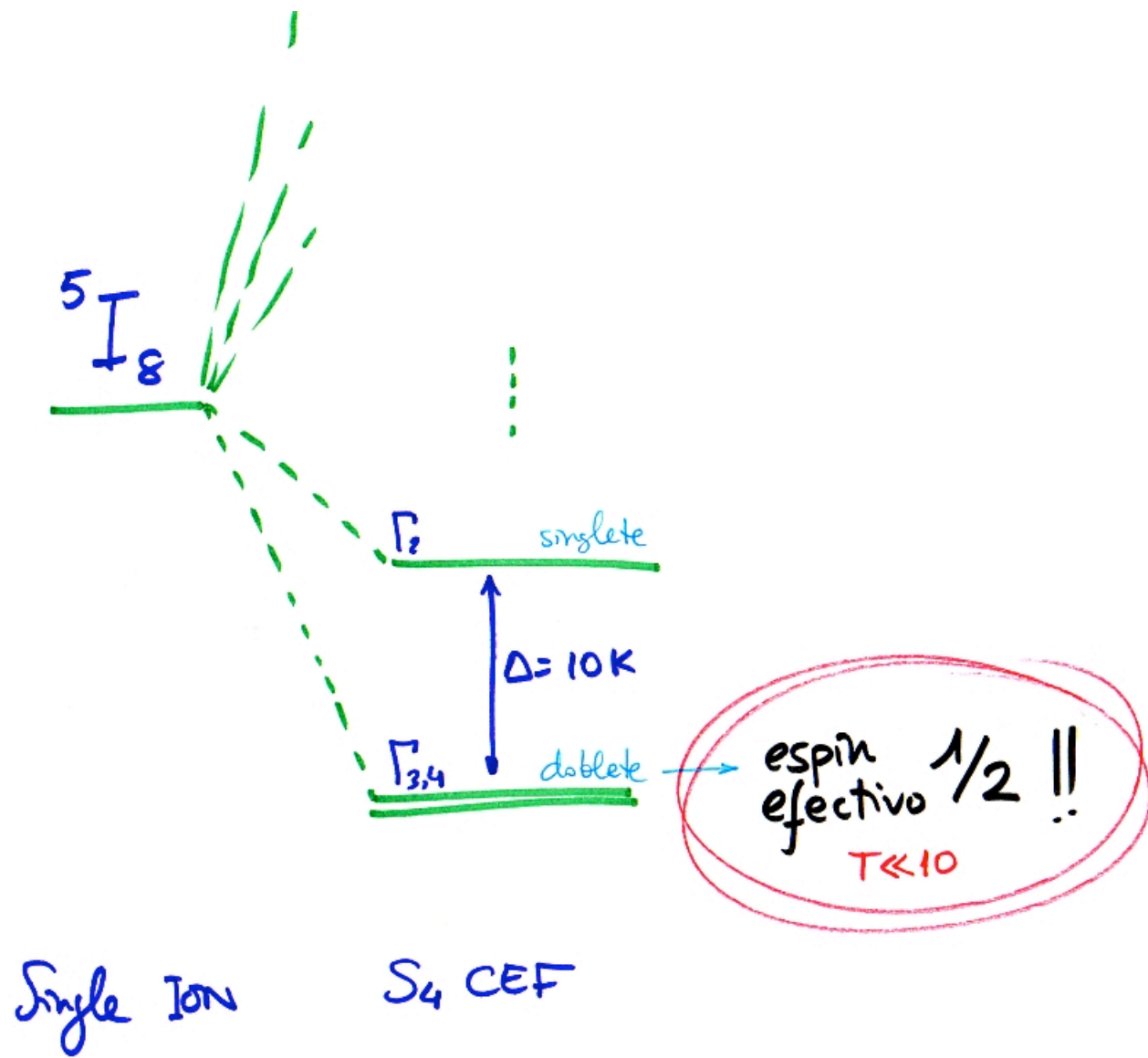
The classical, thermally driven transition in the dipolar-coupled Ising ferromagnet LiHoF_4 ($T_c = 1.53$ K) can be converted into a quantum transition driven by a transverse magnetic field H_t at $T = 0$. The transverse field, applied perpendicular to the Ising axis, introduces channels for quantum relaxation, thereby depressing T_c . We have determined the phase diagram in the H_t - T plane via magnetic susceptibility measurements. The critical exponent, $\gamma = 1$, has a mean-field value in both the classical and quantum limits. A solution of the full mean-field Hamiltonian using the known LiHoF_4 crystal-field wave functions, including nuclear hyperfine terms, accurately matches experiment. [S0031-9007(96)00753-3]



$$H_0^{3+} : 4f^{10}$$



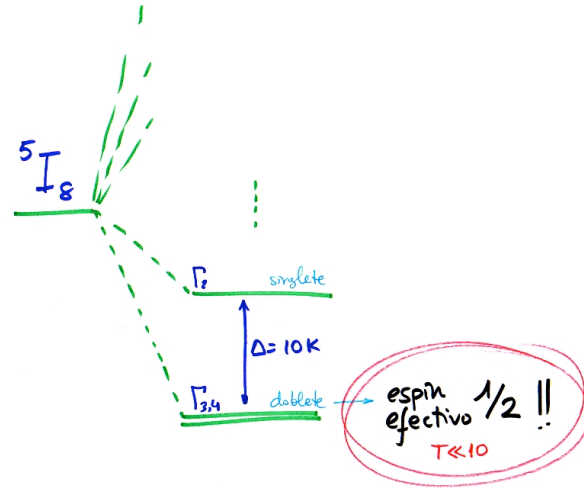




Single ION

S_4 CEF

espin efectivo 1/2 !!
 $T \ll 10$



• ISING ?? Depende del detalle "fino" del CEF

$$|\phi_i\rangle = \sum_{i=-15/2}^{15/2} a_i |6, \frac{3}{2}, \frac{15}{2}, i\rangle ; \sum_{i=-15/2}^{15/2} |a_i|^2 = 1$$

los ais determinan

$$\tilde{g} = \begin{bmatrix} g_{xx} & g_{xy} & g_{xz} \\ g_{yx} & g_{yy} & g_{yz} \\ g_{zx} & g_{zy} & g_{zz} \end{bmatrix}$$

PHYSICAL REVIEW B

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Critical behavior of the magnetic susceptibility of the uniaxial ferromagnet LiHoF₄

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(Received 21 February 1978).

The magnetic susceptibility of two LiHoF₄ single crystals has been measured in the range 1.2–4.2 K. Ferromagnetic order occurs at $T_c = 1.527$ K. Above 2.5 K, the susceptibilities parallel and perpendicular to the fourfold c axis are well interpreted by the molecular-field approximation, taking into account the ground state and the first excited state of Ho³⁺ in the crystal field of S_4 symmetry. The experimental results are consistent with $g_{\parallel} = 13.95$ and $g_{\perp} = 0$ for the ground state. The dipolar contribution to the magnetic interaction is about three times larger than the exchange one. Near T_c , the parallel susceptibility is well described by the classical law with logarithmic corrections theoretically predicted by Larkin and Khmel'mitskii for the uniaxial dipolar ferromagnet or by a power law with a critical-exponent value $\gamma = 1.05$ rather close to 1. The upper limit of the critical region is $(T_{\max} - T_c)/T_c = 1.1 \times 10^{-2}$.

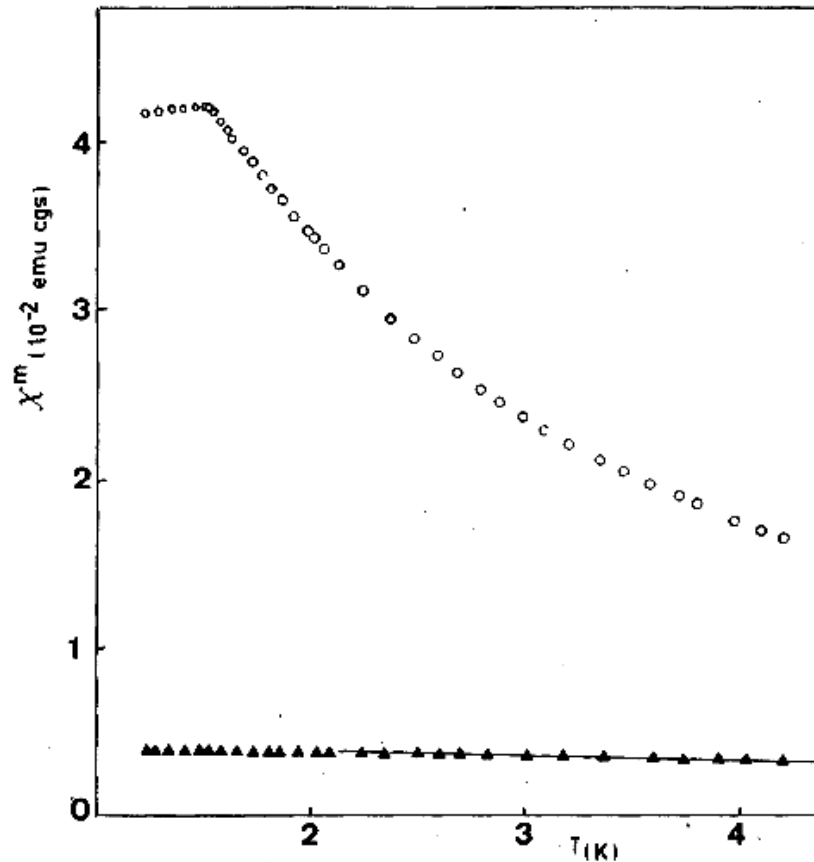


FIG. 1. Experimental parallel susceptibility per gram χ_{\parallel}^m (open circles) and perpendicular susceptibility per gram χ_{\perp}^m (black triangles) vs temperature for the spherical sample. The solid line represents the approximate theoretical law, for $e^{-E_1/kT} \ll 1$: $\chi_{\perp}^m = (n\mu_B^2/4k)(B + Ce^{-E_1/kT})$, with $B = 9.98$, $C = 11.3$, and $E_1/k = 10.4$ K.

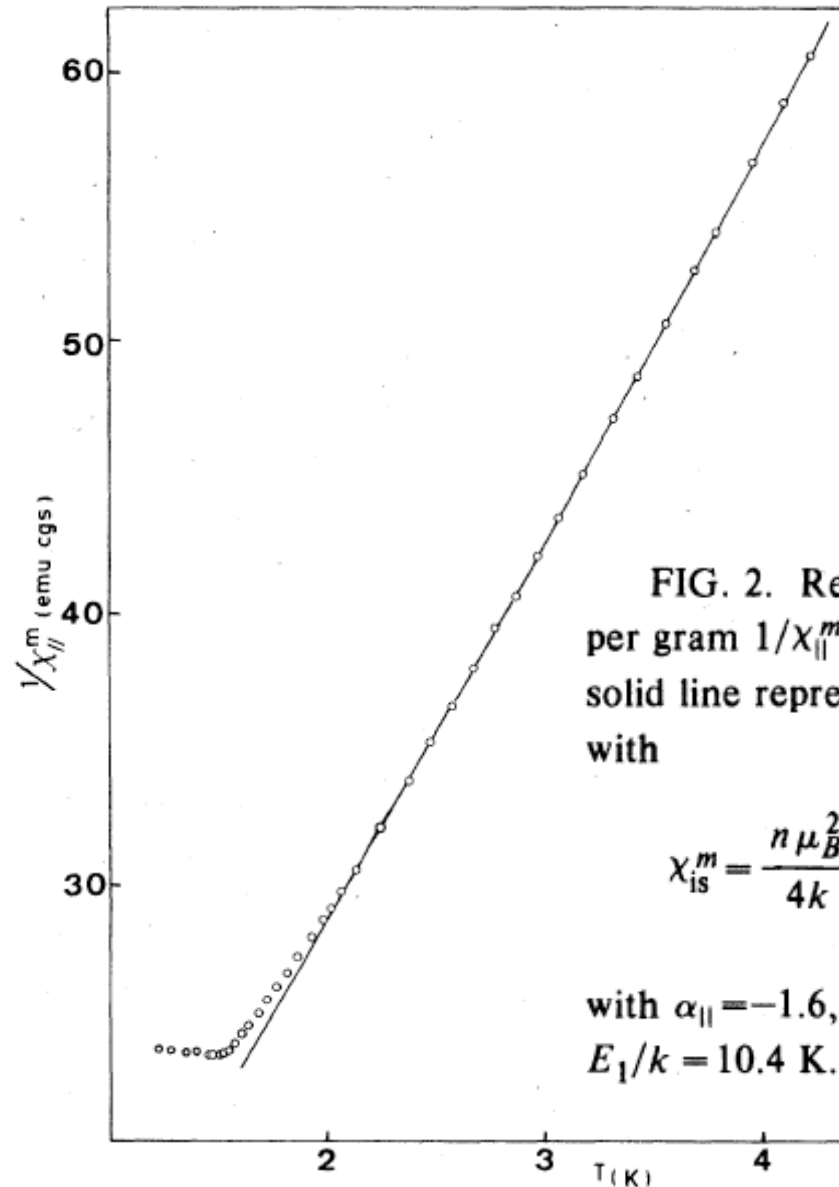


FIG. 2. Reciprocal experimental parallel susceptibility per gram $1/\chi_{||}^m$ vs temperature for a spherical sample. The solid line represents the theoretical curve $1/\chi_{||}^m = 1/\chi_{is}^m - \alpha_{||}$ with

$$\chi_{is}^m = \frac{n \mu_B^2}{4k} \left[\frac{(g_{||}^0)^2 T^{-1} + a_{||}^0 + a_{||}^1 e^{-E_1/kT}}{1 + 0.5 e^{-E_1/kT}} \right]$$

with $\alpha_{||} = -1.6$, $g_{||}^0 = 13.95$, $a_{||}^0 = 0.25$, $a_{||}^1 = 3.3$, and $E_1/k = 10.4$ K.

$$\chi_{\text{isol}}^m = \frac{n \mu_B^2}{4 k_B} \cdot \frac{\overset{\text{GROMAGNETIC RATIO}}{g_{\parallel}^0} T^{-1} + \overset{\text{VAN VLECK}}{a_{\parallel}^0} + \overset{\text{VAN VLECK}}{a_{\parallel}^1} e^{-E_1/k_B T}}{1 + \frac{1}{2} e^{-E_1/k_B T}}$$

$$g_{\parallel}^0 = 13.95 \quad (X)$$

$$g_{\parallel}^0 = 14.1(2) \text{ E.P.R.}$$

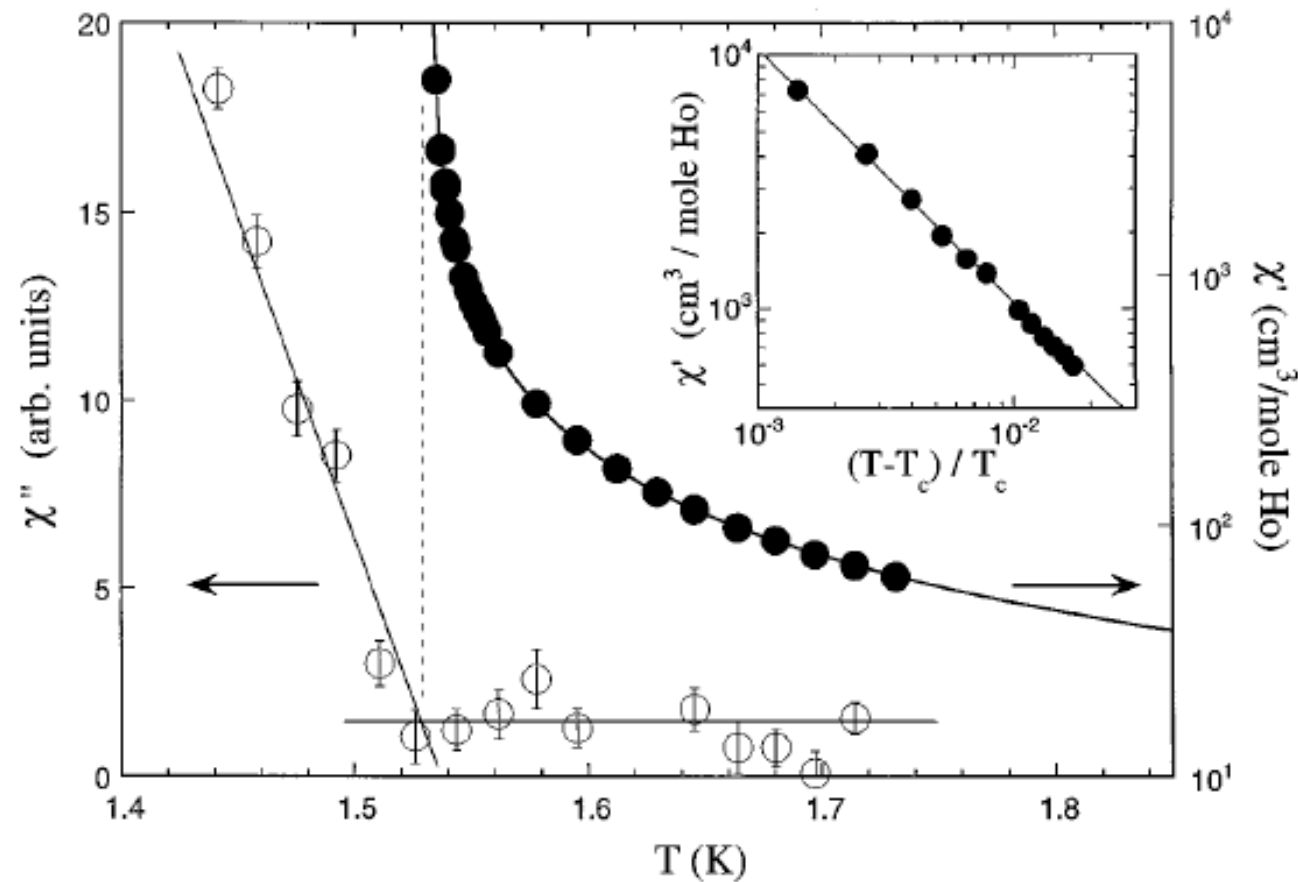
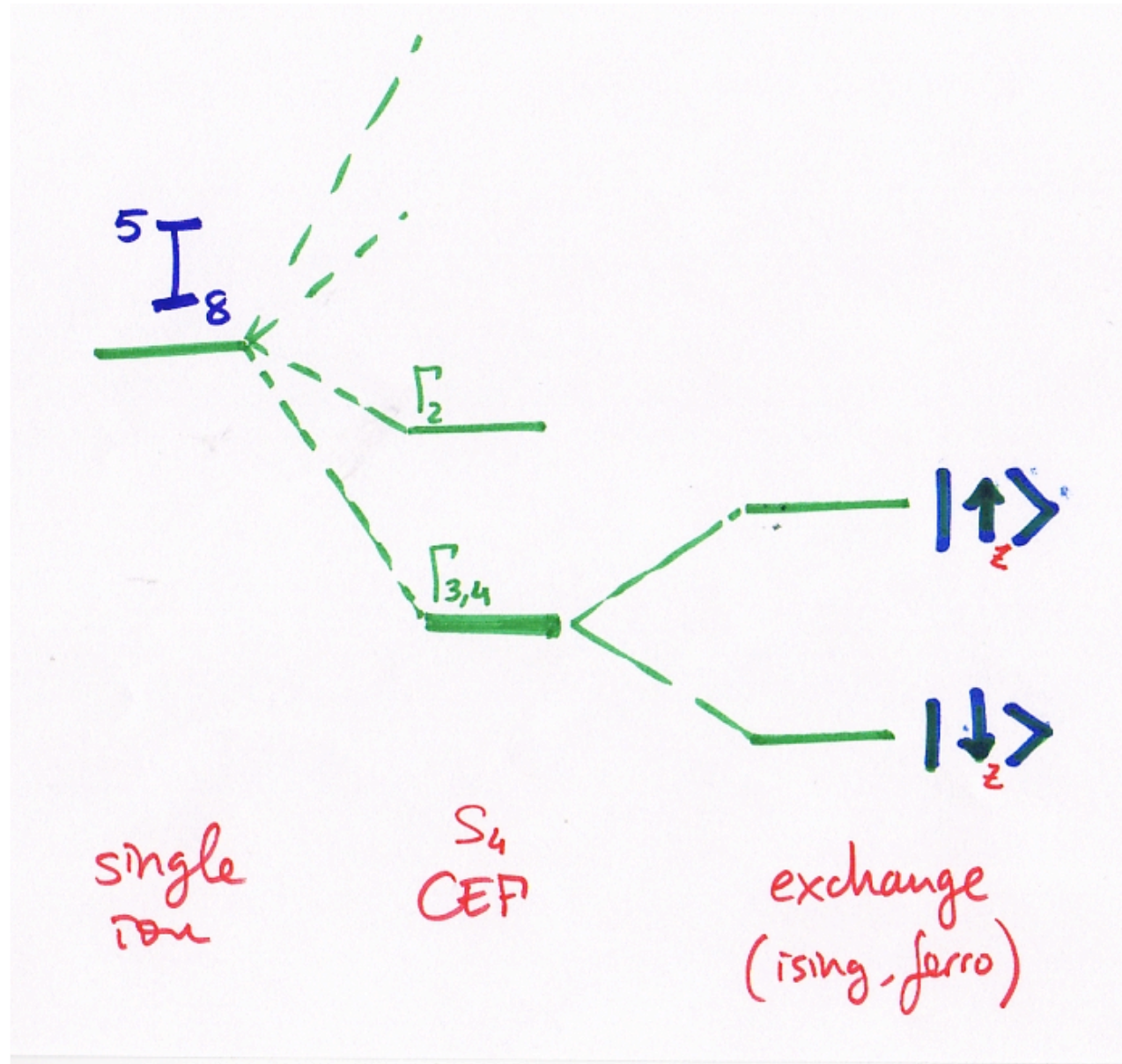
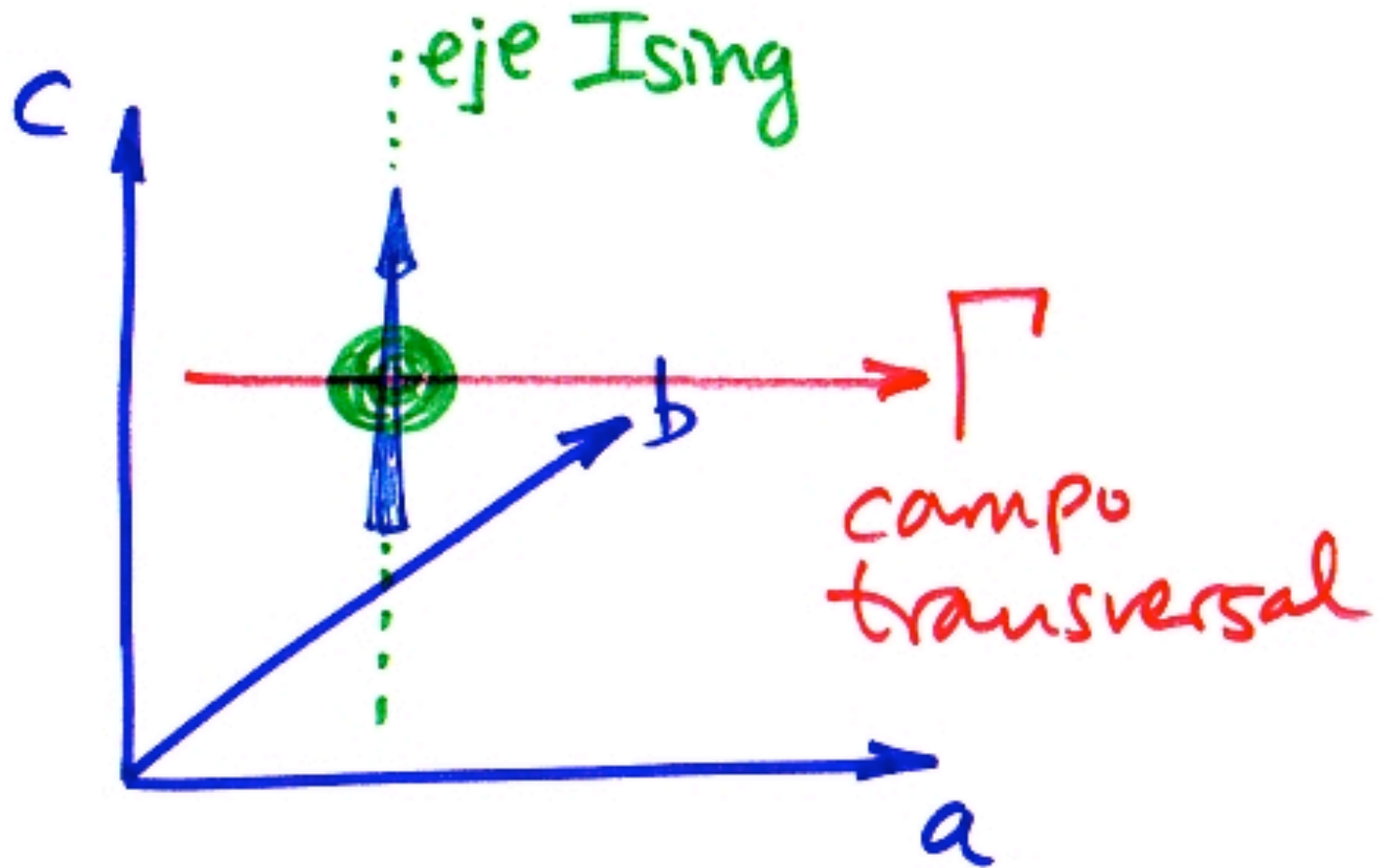
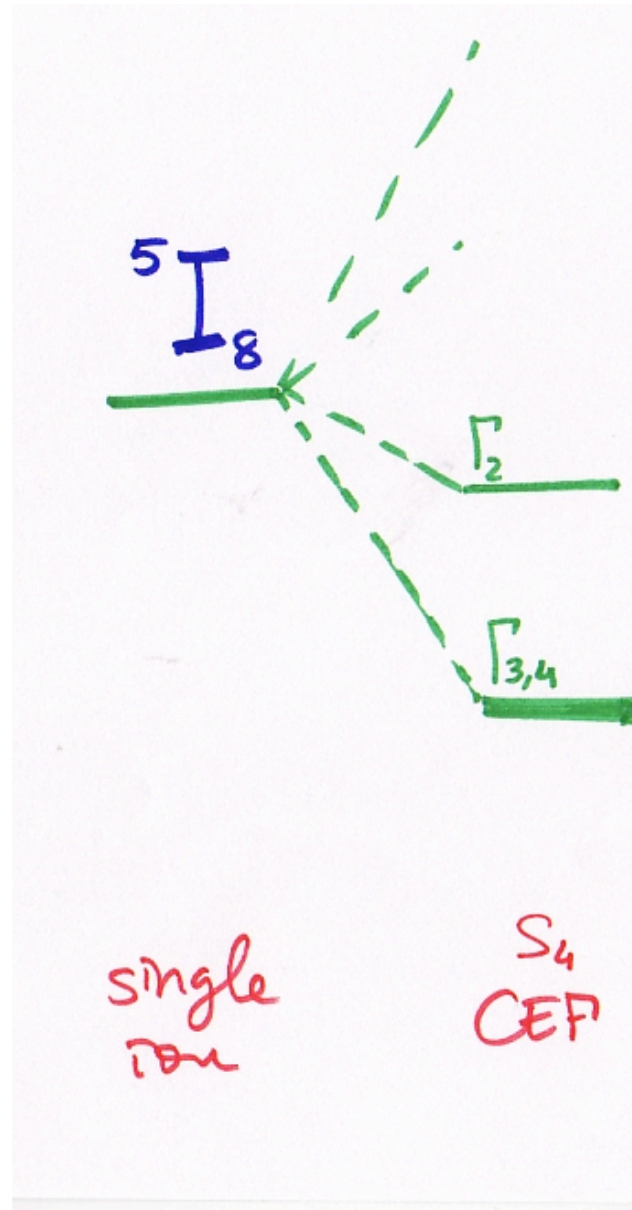


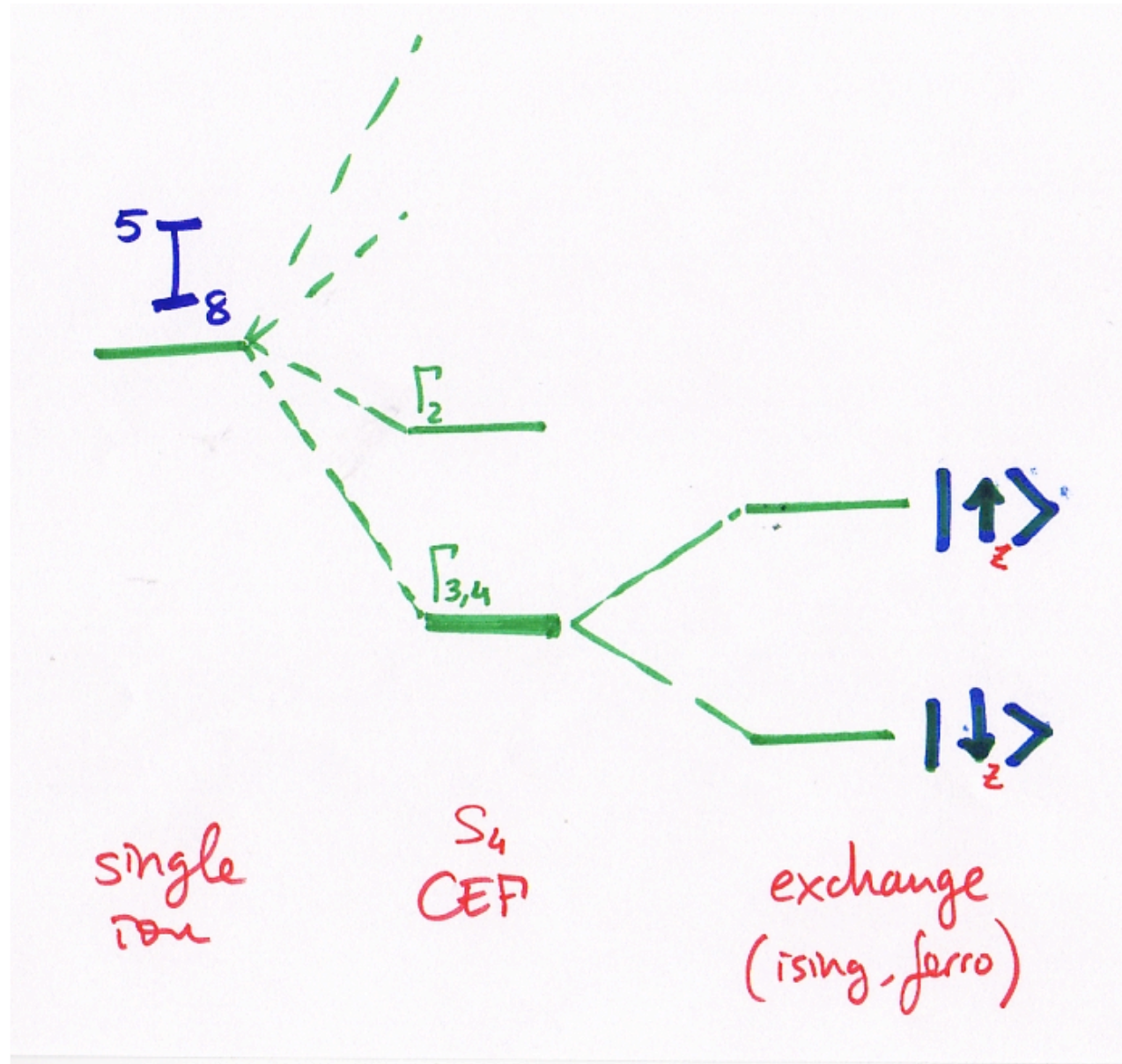
FIG. 1. Divergence of the real part of the magnetic susceptibility (filled circles) and sharp increase in the imaginary part (open circles) at the thermally driven ferromagnetic transition in LiHoF_4 . Inset: Mean-field critical behavior with $\chi' \propto t^{-\gamma}$ and best-fit value $\gamma = 1.00 \pm 0.09$ (line).



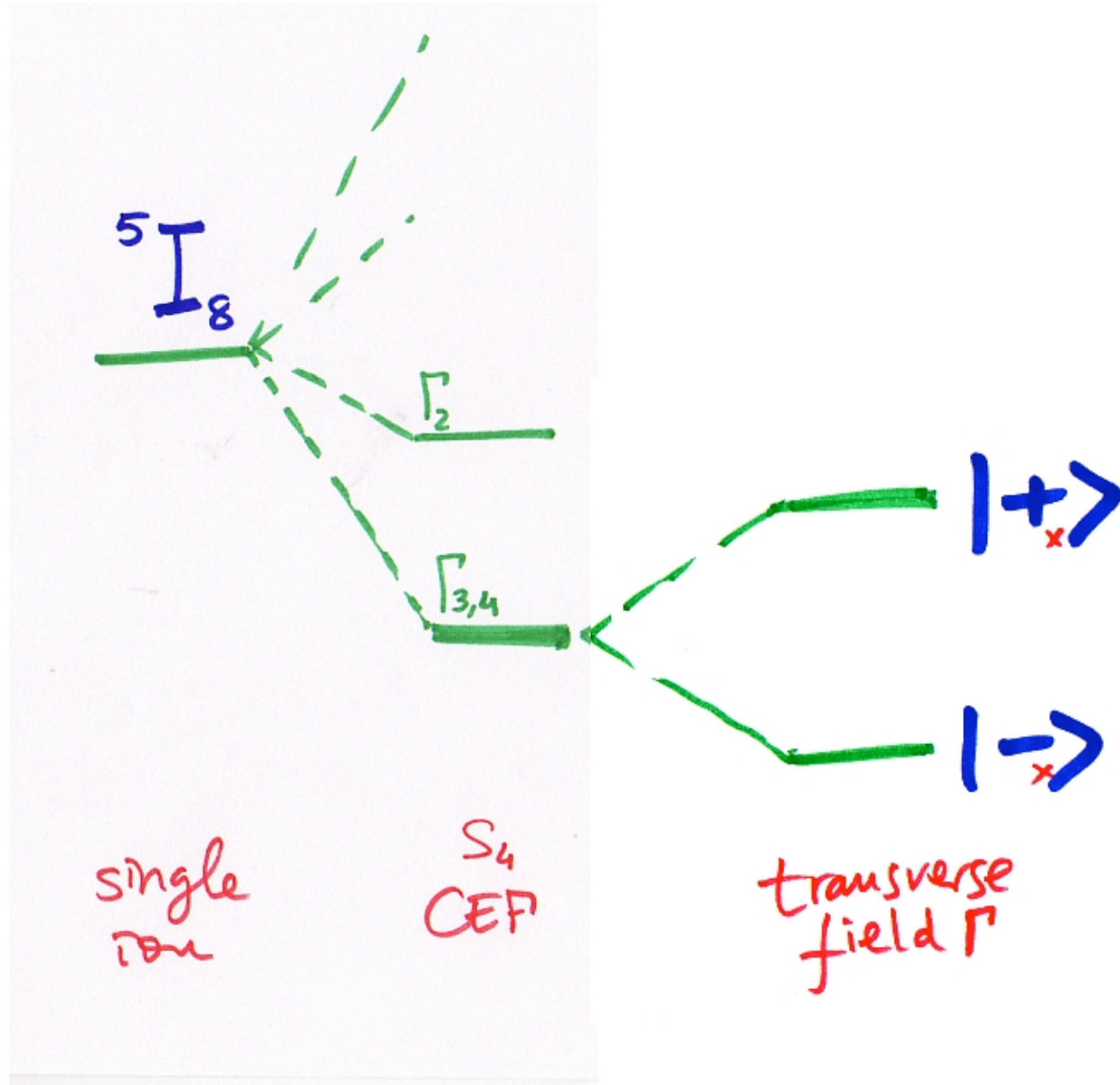


Física de Bajas Temperaturas - Transiciones de Fase





Física de Bajas Temperaturas - Transiciones de Fase



$$|\pm\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow_z\rangle \pm |\downarrow_z\rangle \right)$$

Transición (*de fase cuántica*) de
Orden Clásico Ferromagnético
a **Desorden Cuántico !!**

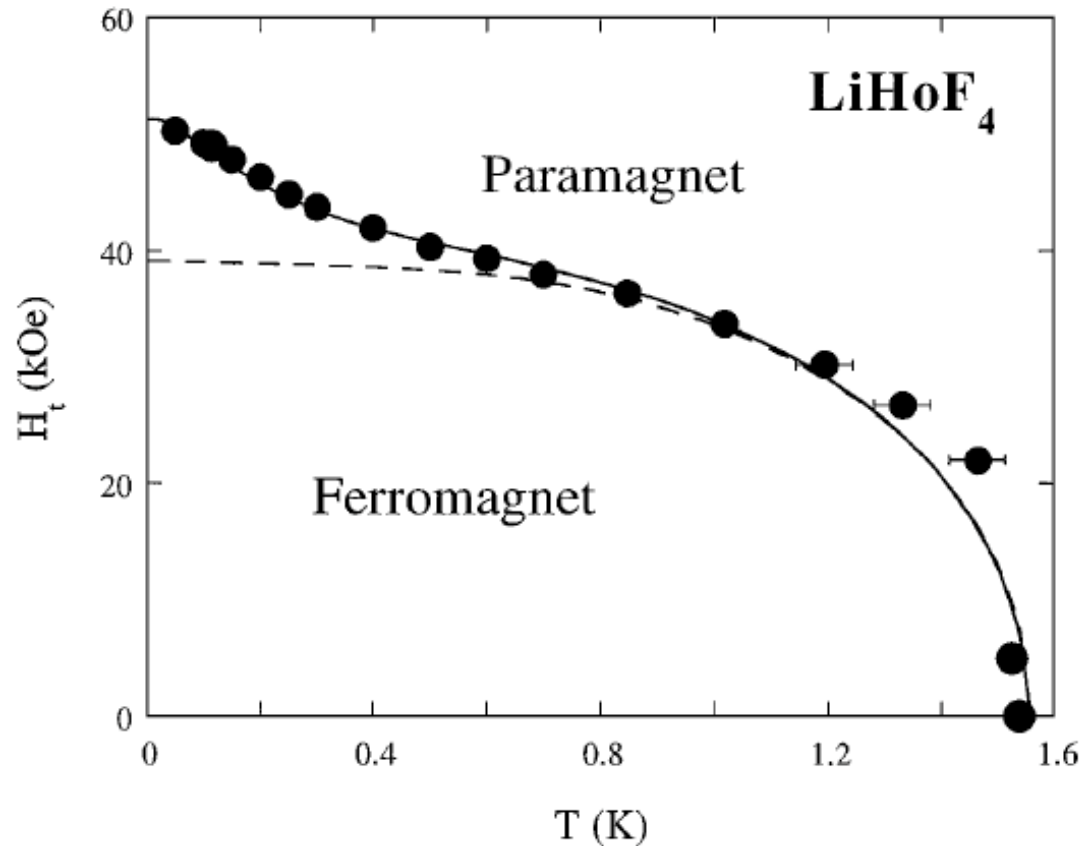
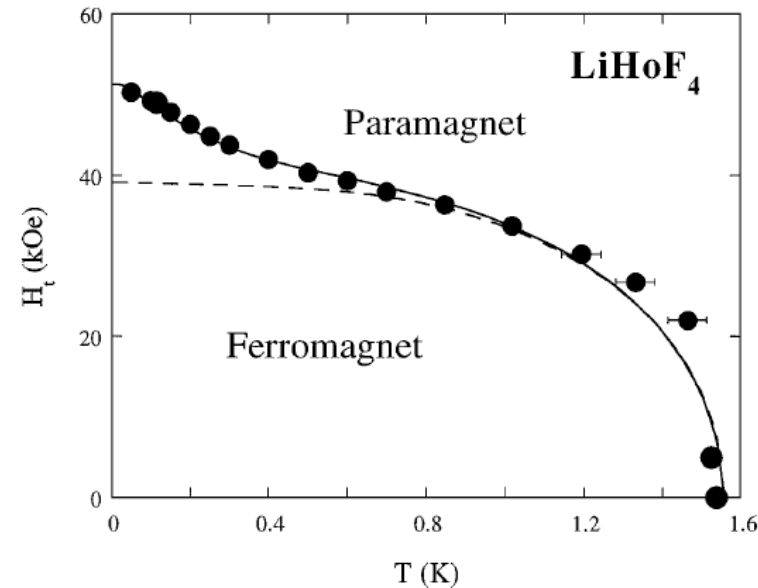


FIG. 3. Experimental phase boundary (filled circles) for the ferromagnetic transition in the transverse field-temperature plane. Dashed line is a mean-field theory including only the electronic spin degrees of freedom; solid line is a full mean-field theory incorporating the nuclear hyperfine interaction [Eq. (2)]. Both theories have the same two fitting parameters.



$$T > 0.6 \text{ K} \quad \text{cotgh} \left(\frac{\Gamma}{2kT_c} \right) = J/\Gamma \quad \text{---}$$

ising ferro; transverse field

$T < 0.6 \text{ K}$ nuclear hyperfine interaction needed

$$\mathcal{H} = V_c - g_{\perp} \mu_B \Gamma \vec{J}_x + A (\vec{I} \cdot \vec{J}) - 2J \langle \vec{J}_z \rangle \vec{J}_z$$

$\uparrow_{I=7/2}$

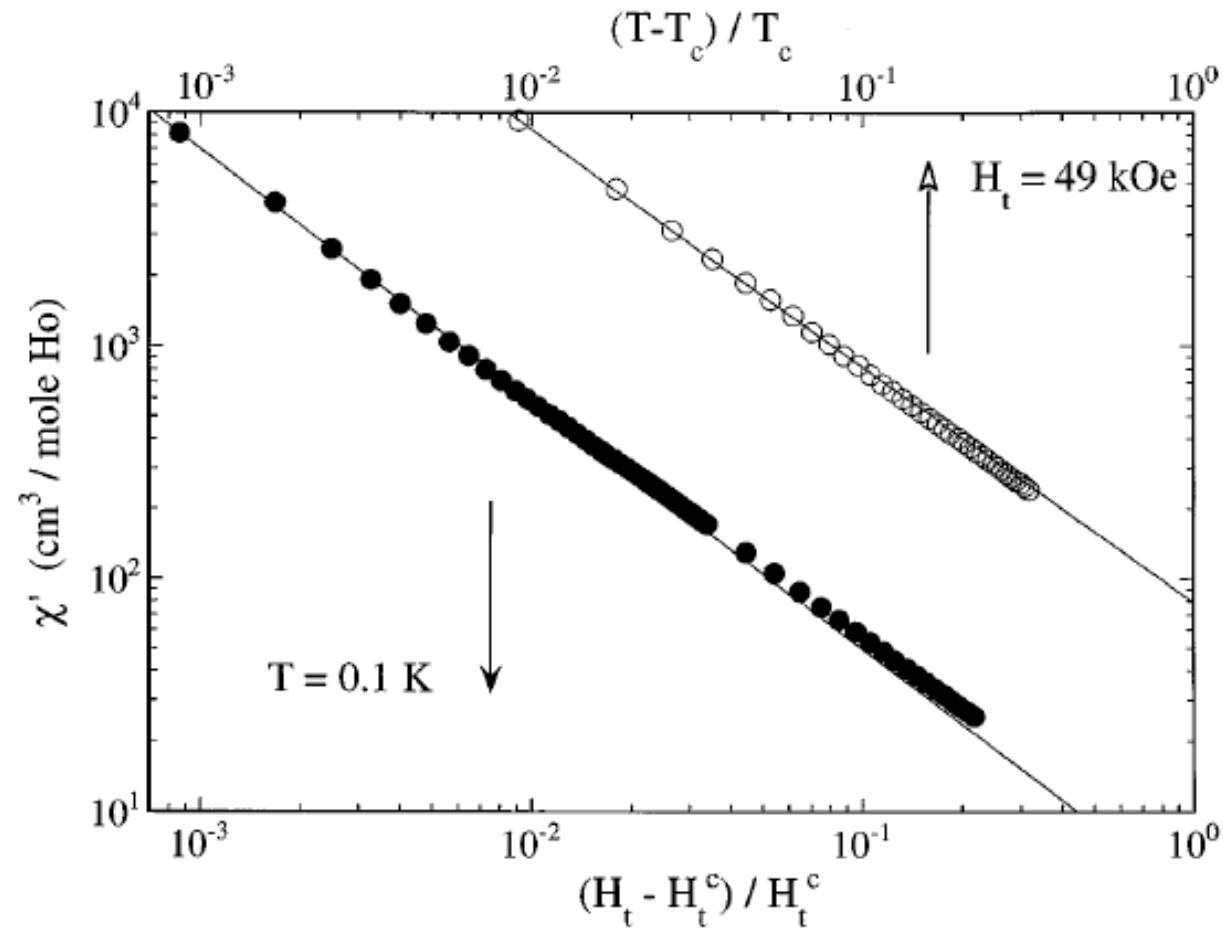


FIG. 2. Mean-field critical behavior of the magnetic susceptibility in the $T \rightarrow 0$ limit as functions of reduced temperature (open circles, $T_c = 0.114$ K, $H_t = 49.0$ kOe) and reduced transverse field (filled circles, $H_t^c = 49.3$ kOe, $T = 0.100$ K).

We find $\gamma = 1$ within error bars at all temperatures studied, down to the lowest temperature probed, $T = 0.050$ K or 3% of $T_c(H_t = 0)$. Hence, we conclude that the critical behavior at the quantum ferromagnetic transition in LiHoF_4 retains its mean-field character. This observation verifies the theoretical prediction [11] that the $T = 0$ critical exponents of a d -dimensional Ising model in transverse field are equivalent to those of a $(d + 1)$ -dimensional Ising model in zero transverse field. Studies

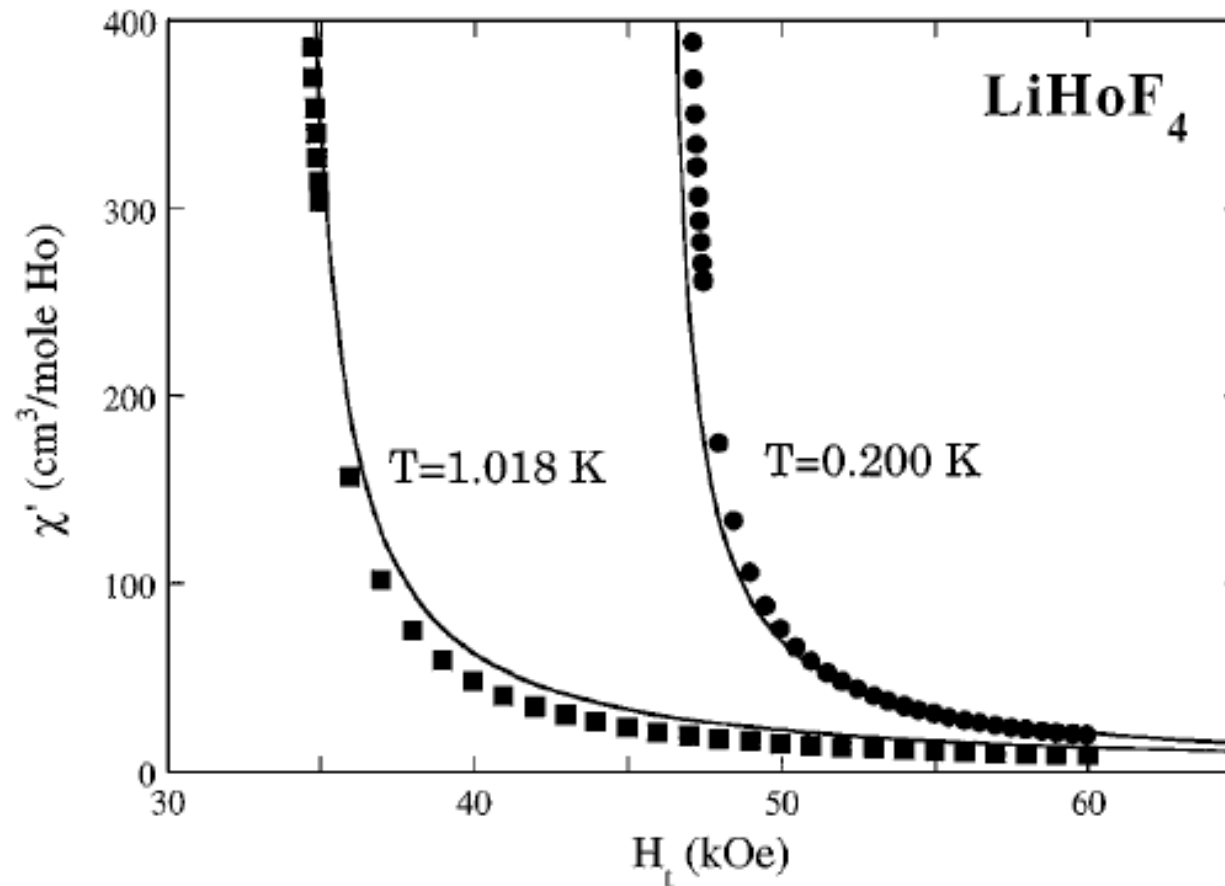


FIG. 4. Transverse field dependence of the susceptibility in the paramagnet for two temperatures. Solid line is a first principles calculation with parameters fixed by the fit to the phase boundary of Fig. 3.

PRL **95**, 227202 (2005)

PHYSICAL REVIEW LETTERS

week ending
25 NOVEMBER 2005

Long-Range Ferromagnetism of Mn_{12} Acetate Single-Molecule Magnets under a Transverse Magnetic Field

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(Received 10 February 2005; revised manuscript received 23 May 2005; published 21 November 2005)

We use neutron diffraction to probe the magnetization components of a crystal of Mn_{12} single-molecule magnets. Each of these molecules behaves, at low temperatures, as a nanomagnet with spin $S = 10$ and strong anisotropy along the crystallographic c axis. The application of a magnetic field H_{\perp} perpendicular to c induces quantum tunneling between opposite spin orientations, enabling the spins to attain thermal equilibrium. For $T \approx 0.9(1)$ K, this equilibrium state shows spontaneous magnetization, indicating the onset of ferromagnetism. These long-range magnetic correlations nearly disappear for $\mu_0 H_{\perp} \approx 5.5$ T, possibly suggesting the existence of a quantum critical point.

DOI: [10.1103/PhysRevLett.95.227202](https://doi.org/10.1103/PhysRevLett.95.227202)

PACS numbers: 75.45.+j, 75.30.Kz, 75.50.Xx

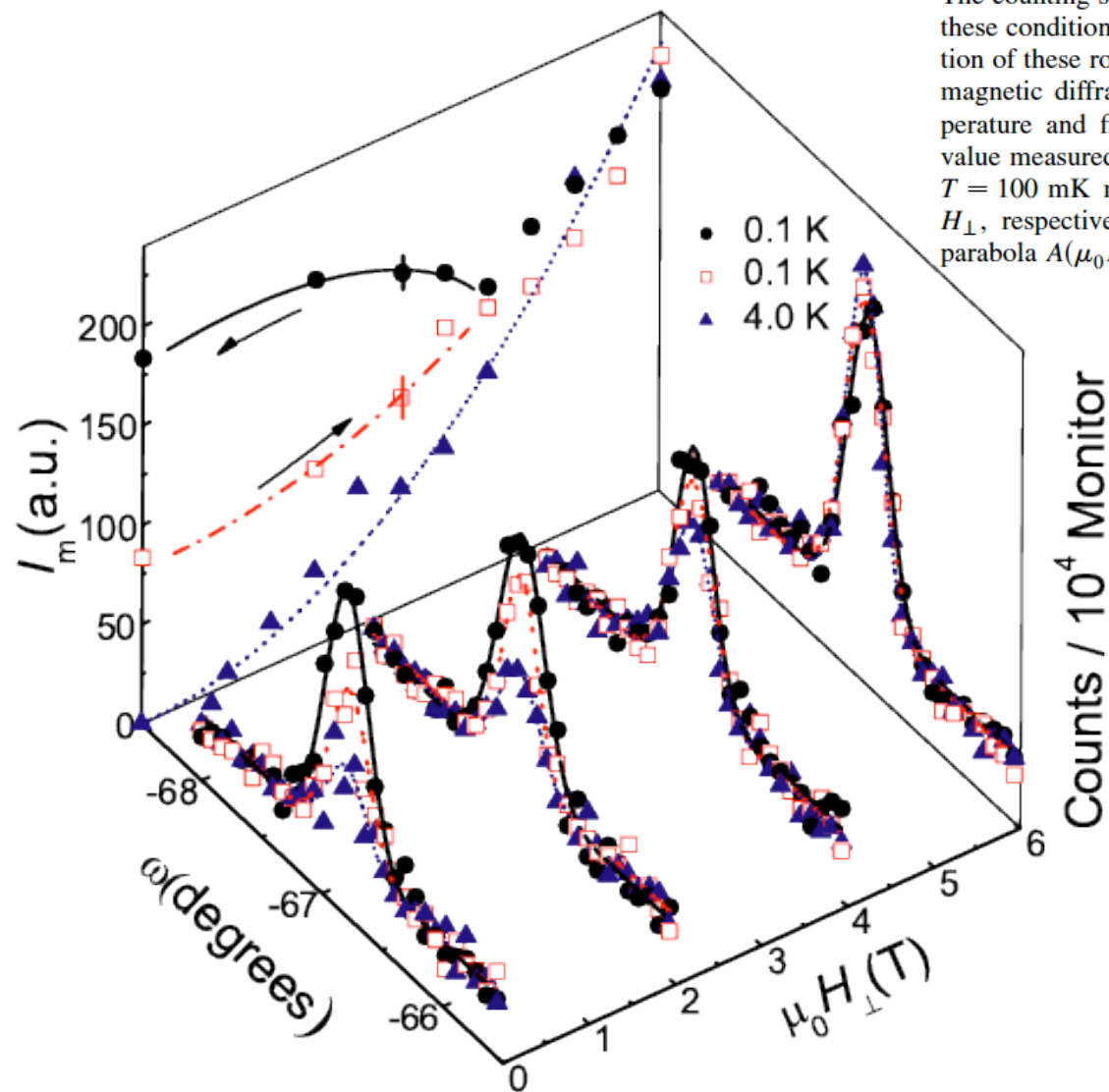


FIG. 1 (color online). Rocking curves for the $(\bar{2}\bar{2}0)$ reflection measured at two different temperatures and four magnetic fields. The counting statistics are typical for such a small crystal under these conditions. The lines are Gaussian fits. Numerical integration of these rocking curves gives the diffracted intensity I . The magnetic diffraction intensities I_m were obtained at each temperature and field by subtracting from the total intensity the value measured at 4 K and $\mu_0 H_{\perp} = 0$. \blacktriangle , $T = 4$ K; \square and \bullet , $T = 100$ mK measured while increasing and then decreasing H_{\perp} , respectively. The dotted line is a least-squares fit to a parabola $A(\mu_0 H_{\perp})^2$.

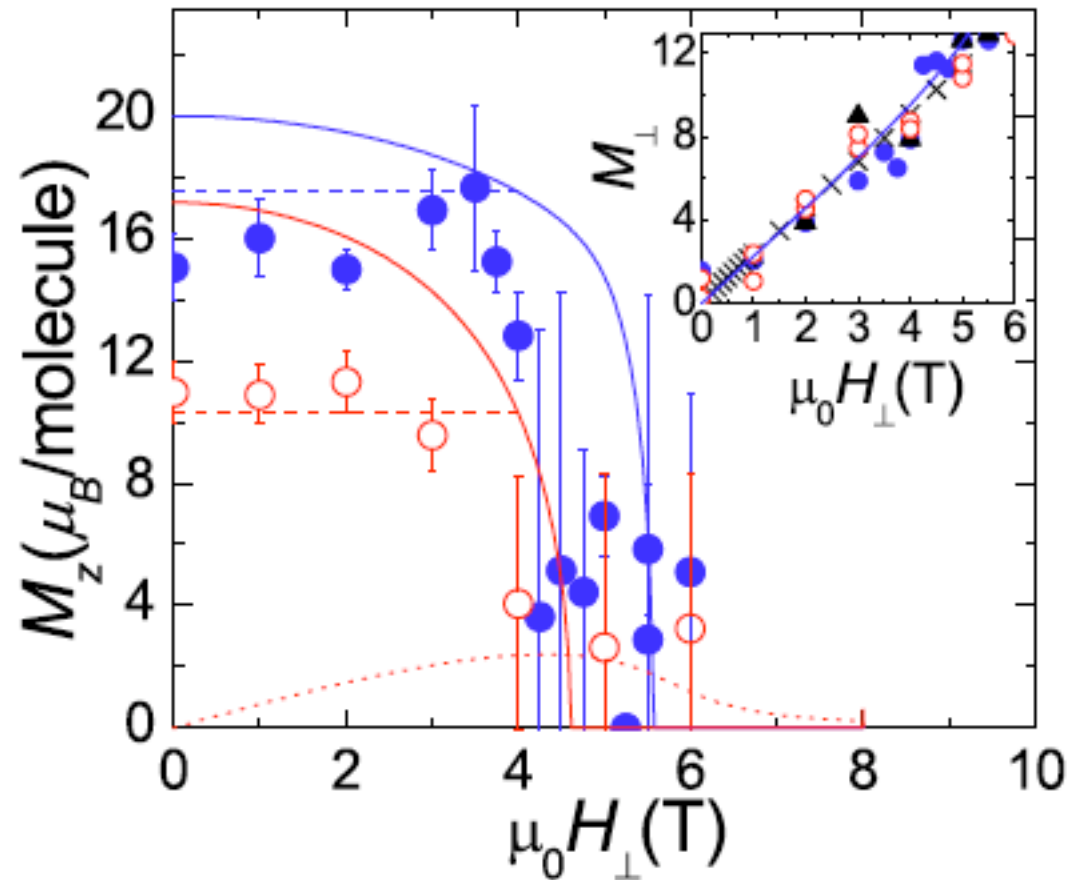
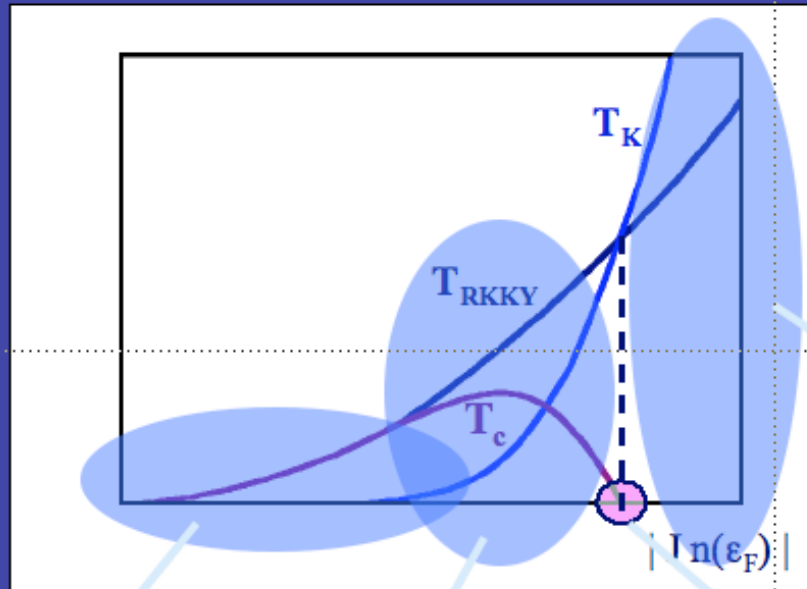


FIG. 2 (color online). Longitudinal magnetization M_z of Mn_{12} acetate measured while decreasing the transverse magnetic field from 6 T. \bullet and \circ are for $T = 47$ and 600 mK, respectively.

Diagrama de Doniach



$$T_{RKKY} \propto (J n(\epsilon_F))^2$$

$$T_K \propto e^{-\left(\frac{1}{|J| n(\epsilon_F)}\right)}$$

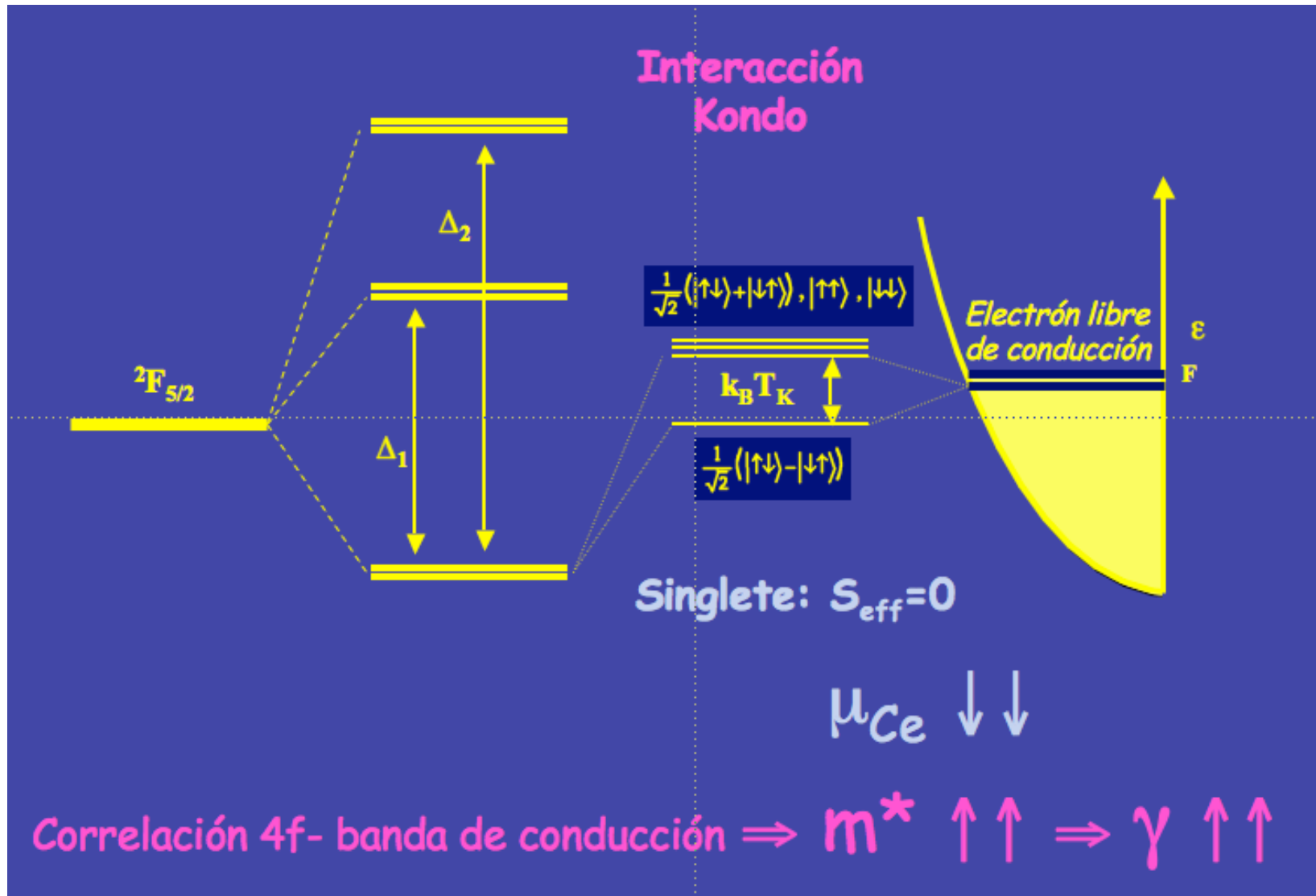
$T_{RKKY} \gg T_K$
El sistema se ordena

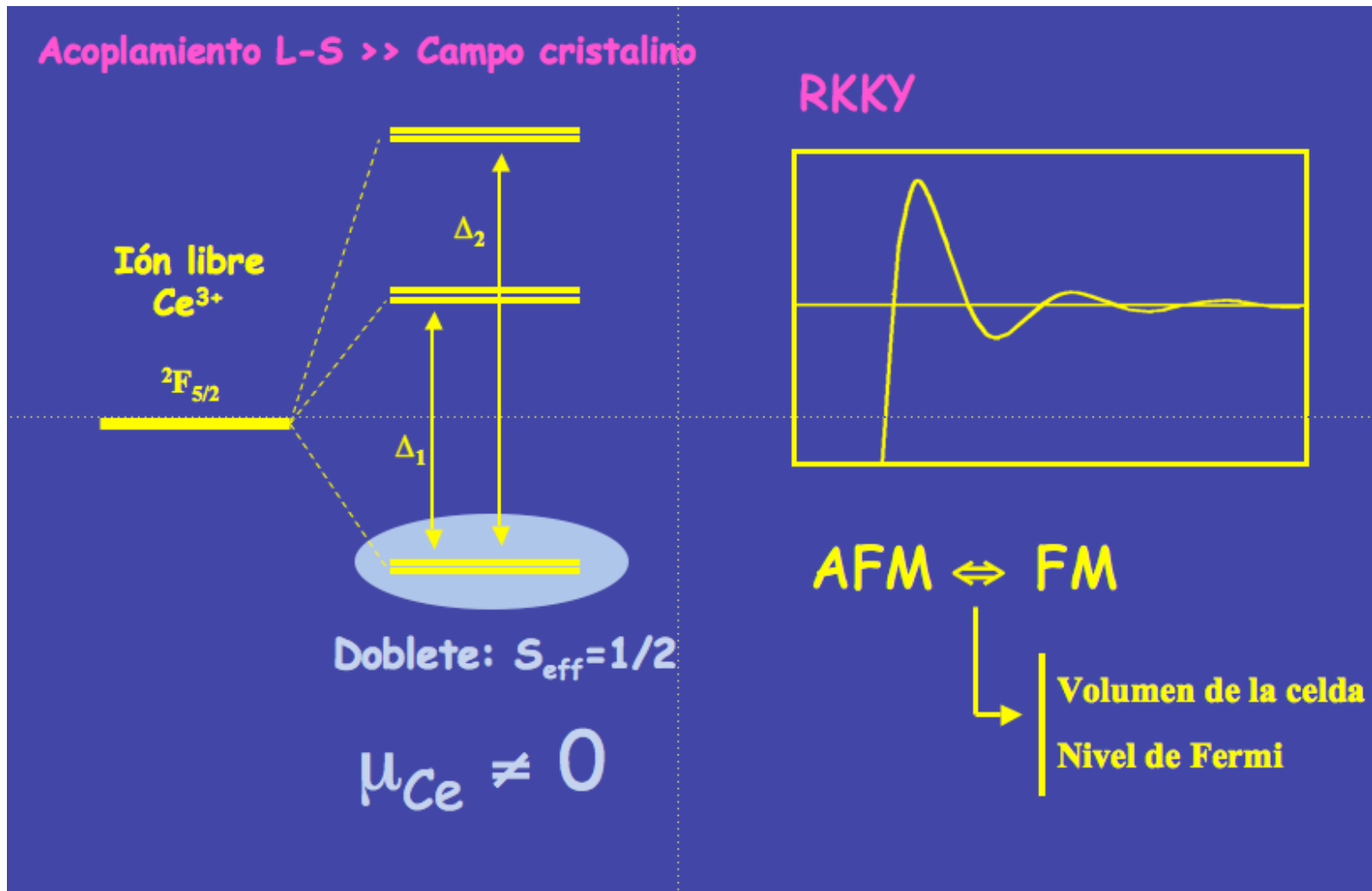
$T_{RKKY} \approx T_K$
Momento magnético promedio reducido
El sistema se puede ordenar

$T_C \rightarrow 0$
Desaparición del magnetismo
Hibridación 4f-banda de conducción muy fuerte

$T_{RKKY} < T_K$
Estado fundamental no magnético

} NFL



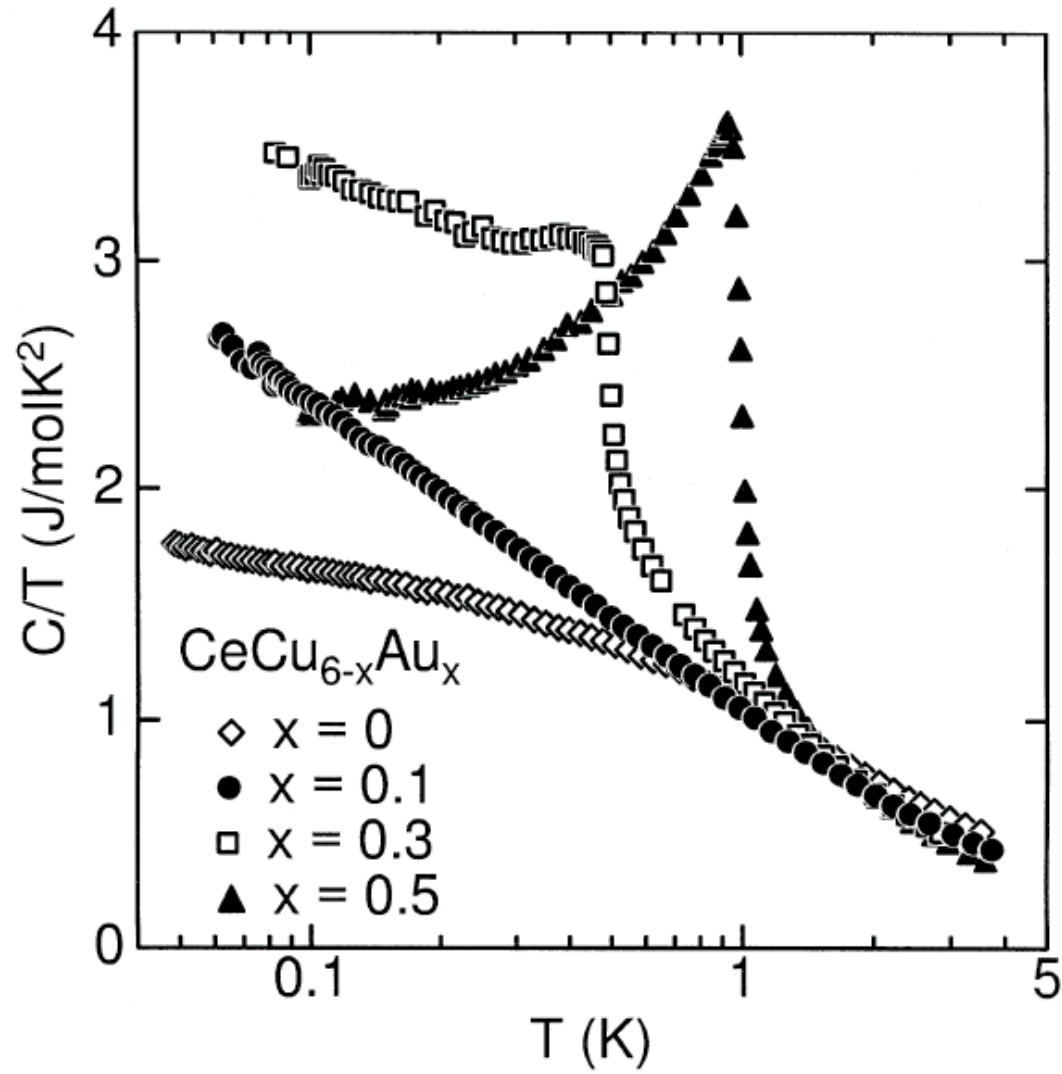


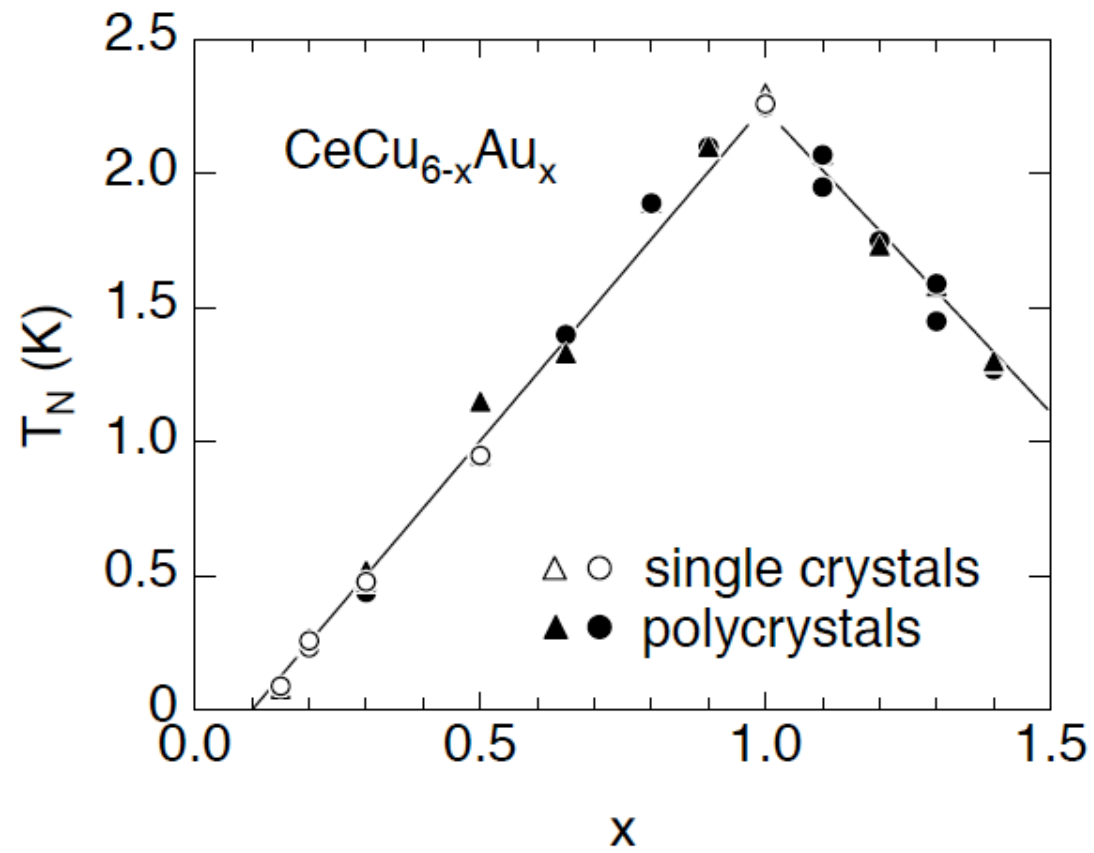
Quantum phase transitions in strongly correlated electron systems

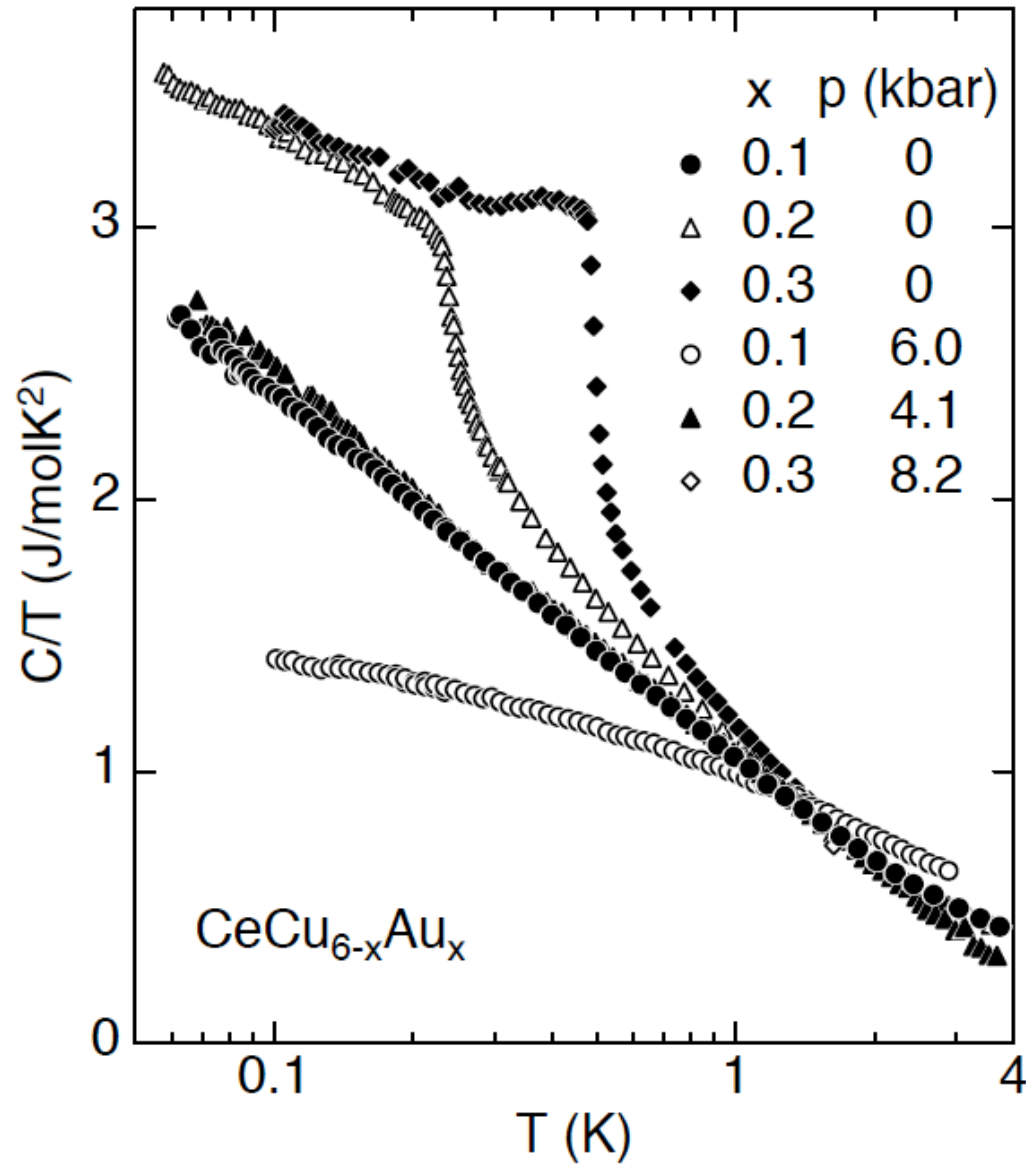
Hilbert v. Löhneysen

Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany

A number of strongly correlated electron systems, notably heavy-fermion alloys, exhibit remarkable deviations from Fermi-liquid behavior at low temperatures. We focus on $\text{CeCu}_{6-x}\text{Au}_x$ and related alloys which have been studied most thoroughly. Non-Fermi-liquid behavior, i.e. unusual temperature dependencies of the specific heat, magnetic susceptibility, and electrical resistivity is found at the critical concentration where a quantum phase transition occurs from a nonmagnetic ground state (i.e. CeCu_6) to a magnetically ordered state ($x > 0.1$). This transition can also be tuned by external pressure, but tuning by an applied magnetic field leads to different behavior.







PHYSICAL REVIEW B **71**, 134401 (2005)**Magnetic ground state of CeNi_{1-x}Cu_x: A calorimetric investigation**

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(Received 8 November 2004; published 6 April 2005)

CeNi_{1-x}Cu_x is a substitutional magnetic system where the interplay of the different magnetic interactions leads to the disappearance of the long-range magnetic order on the CeNi side. The existence of inhomogeneities (spin clusters or phase coexistence) has been previously detected by magnetization and muon spin relaxation (μ SR) spectroscopy measurements. These inhomogeneities are always observed regardless of the different preparation methods and must, then, be considered as intrinsic. We present a detailed specific heat study in a large temperature range of 0.2 to 300 K. The analysis of these data, considering also previous neutron scattering, magnetic characterization, and μ SR results, allows us to present a convenient description of the system as inhomogeneous on the nanometric scale. Two regimes are detected in the compositional range depending on the dominant Ruderman-Kittel-Kasuya-Yosida or Kondo interactions. We propose that the long-range magnetic order at low temperatures is achieved by a percolative process of magnetic clusters that become static below the freezing temperature T_f . In this scenario the existence of a quantum critical point at the magnetic-nonmagnetic crossover must be discarded. This situation should be considered as an example for other substitutional compounds with anomalous magnetic or superconducting properties.

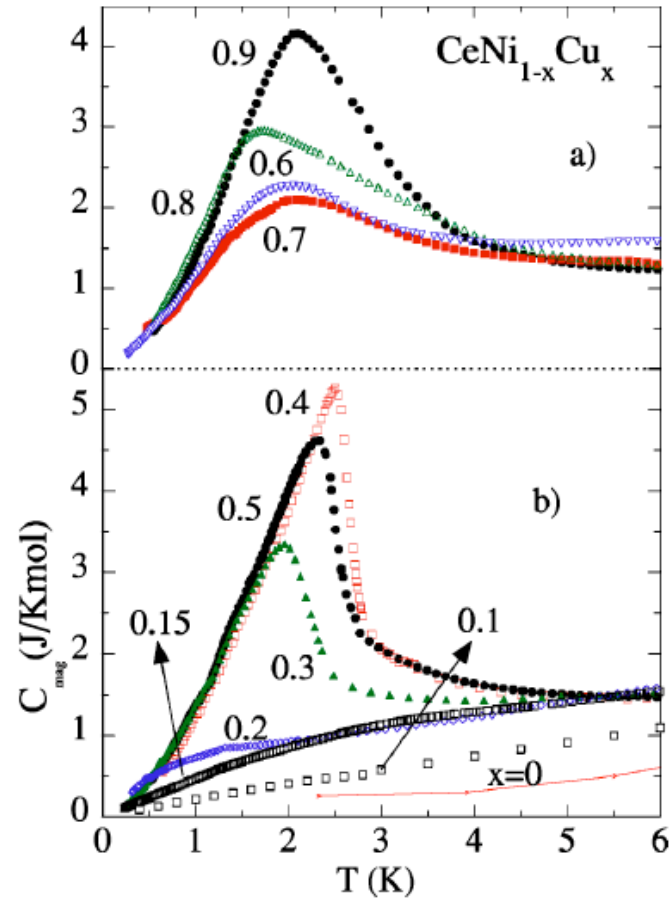


FIG. 5. C_{mag} versus temperature in the low-temperature regime plotted separately for the two composition regions defined: (a) $0.9 \geq x \geq 0.6$ or region where the system evolves from AFM to FM ground state; (b) $x \leq 0.6$ or region where hybridization effects and disorder are predominant (for details see text).

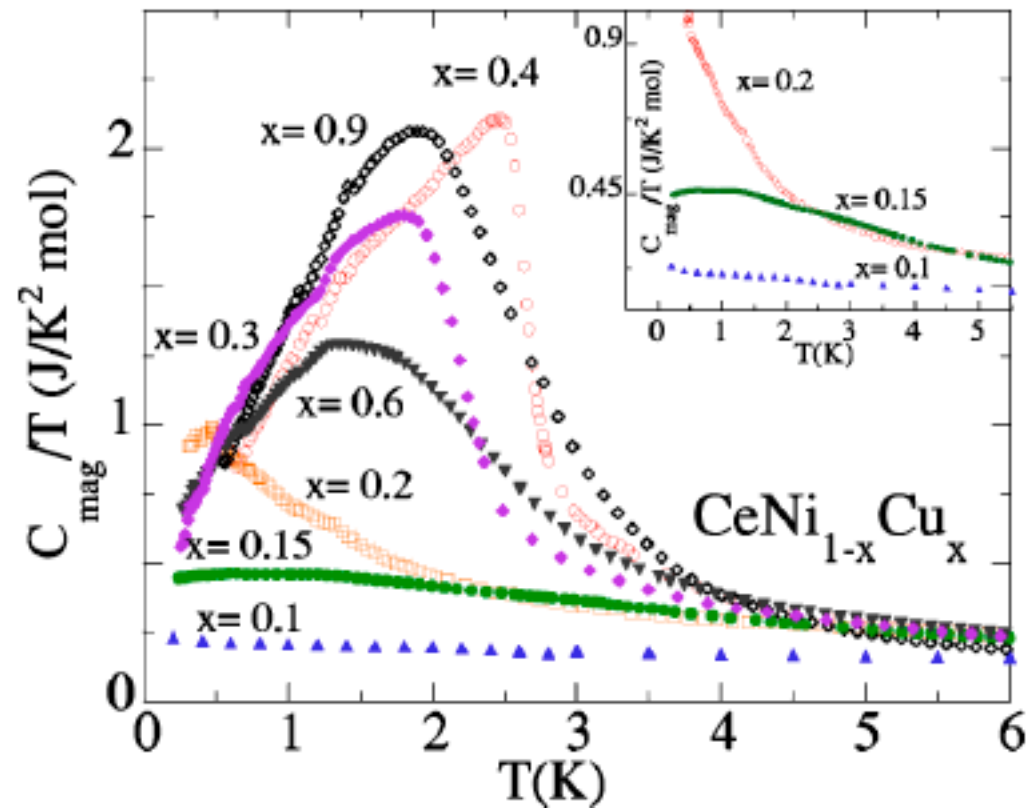


FIG. 6. C_{mag}/T vs T representation of the specific heat for $\text{CeNi}_{1-x}\text{Cu}_x$ in the compositions studied. The inset shows the variation for the compounds near the magnetic-nonmagnetic crossover $x=0.1, 0.15,$ and 0.2 .

studies by both macroscopic (ac and dc measurements¹⁴) and microscopic (μ SR) techniques¹³ in the compositions around $x=0.2$ revealed that the magnetic moments are not yet exhausted. However, long-range magnetic order, if it exists, cannot be detected by neutron diffraction (within the resolution of the available experiments) since we are dealing with very reduced values of the magnetic moment. Both experiments point toward some kind of short-range ordered states and reveal evidence of spin-glass arrangements even for the $x=0.1$ compound.¹⁵ Thus, on the basis of all these results we have to discard an intrinsic electronic effect leading to a NFL or quantum phase transition around the $x=0.2$ compound. The divergence in C_{mag}/T could be related to the existence of a small anomaly at lower temperatures as was found at very low temperature in ac susceptibility measurements.¹⁴

.....

How 'spin ice' freezes

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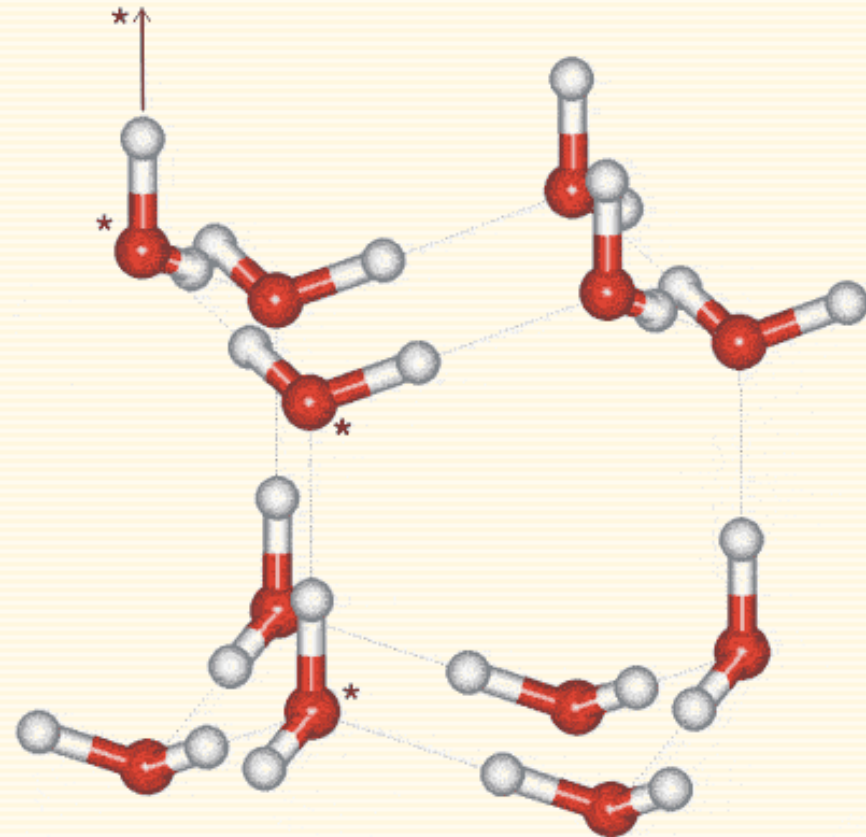
The large degeneracy of states resulting from the geometrical frustration of competing interactions is an essential ingredient of important problems in fields as diverse as magnetism¹, protein folding² and neural networks³. As first explained by Pauling⁴, geometrical frustration of proton positions is also responsible for the unusual low-temperature thermodynamics of ice and its measured 'ground state' entropy⁵. Recent work has shown that the geometrical frustration of ice is mimicked by $\text{Dy}_2\text{Ti}_2\text{O}_7$, a site-ordered magnetic material in which the spins reside on a lattice of corner-sharing tetrahedra where they form an unusual magnetic ground state known as 'spin ice'^{6–13}. Here we identify a cooperative

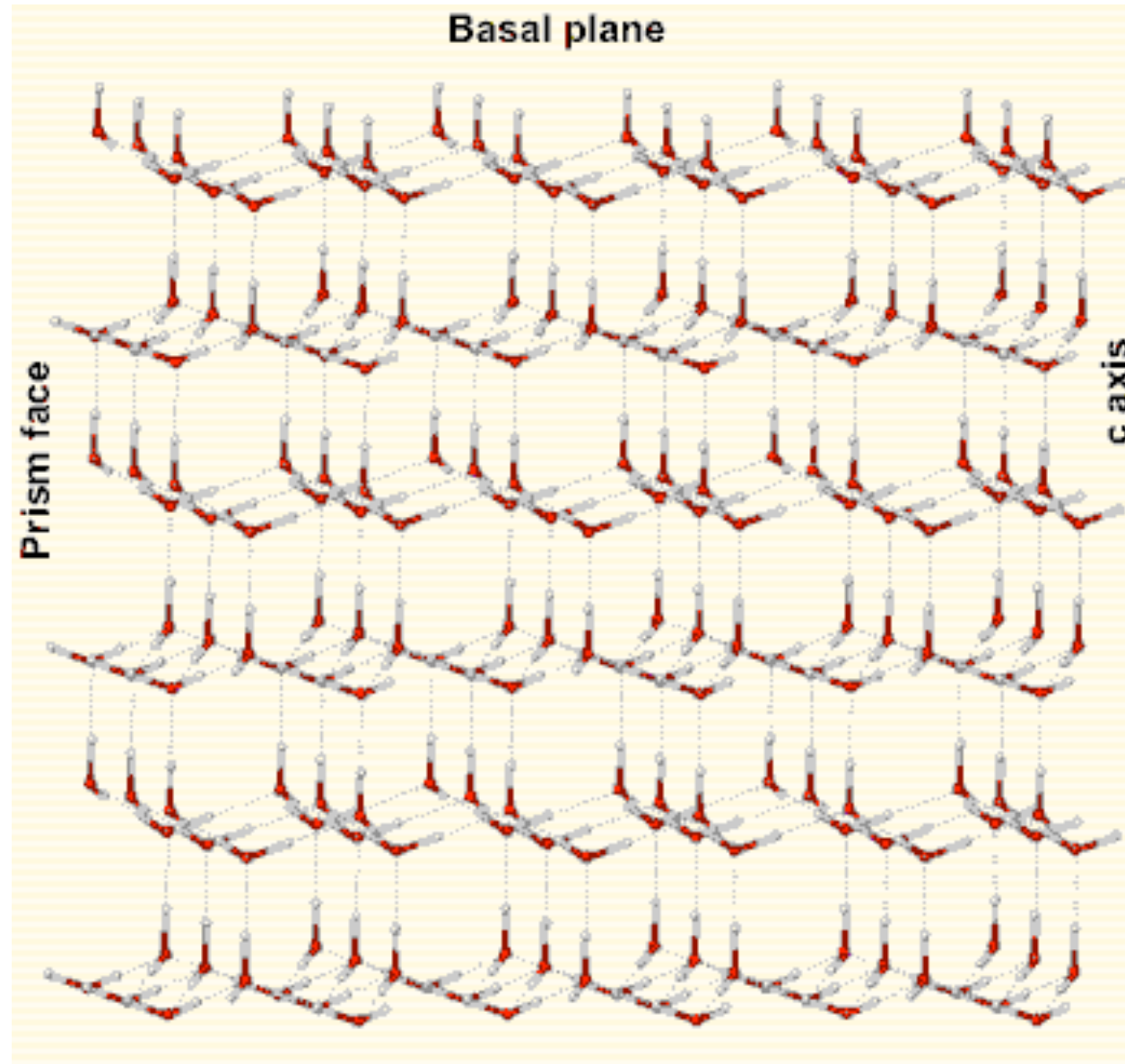
Hexagonal Ice (Ice Ih)

Hexagonal ice (ice Ih) is the form of all natural snow and ice on Earth (see [Phase Diagram](#)), as evidenced in the six-fold symmetry in ice crystals grown from water vapor (*i.e.* [snow flakes](#)).

Hexagonal ice (Space group $P6_3/mmc$, **194**;

Laue class symmetry $6/mmm$; analogous to β -tridymite silica) possesses a fairly open low-density structure, where the packing efficiency is low ($\sim 1/3$) compared with simple cubic ($\sim 1/2$) or face centered cubic ($\sim 3/4$) structures¹ (and in contrast to face centered cubic close packed solid hydrogen sulfide). The crystals may be thought of as consisting of sheets lying on top of each other. The [basic structure](#) consists of a hexameric box where planes consist of chair-form hexamers (the two horizontal planes, opposite) or boat-form hexamers (the three vertical planes, opposite). In this diagram the hydrogen bonding is shown ordered whereas in reality it is random.² The water molecules have a staggered arrangement of hydrogen bonding with respect to three of their neighbors, in the plane of the chair-form hexamers. The fourth neighbor (shown as vertical links opposite) has an eclipsed arrangement of hydrogen bonding.

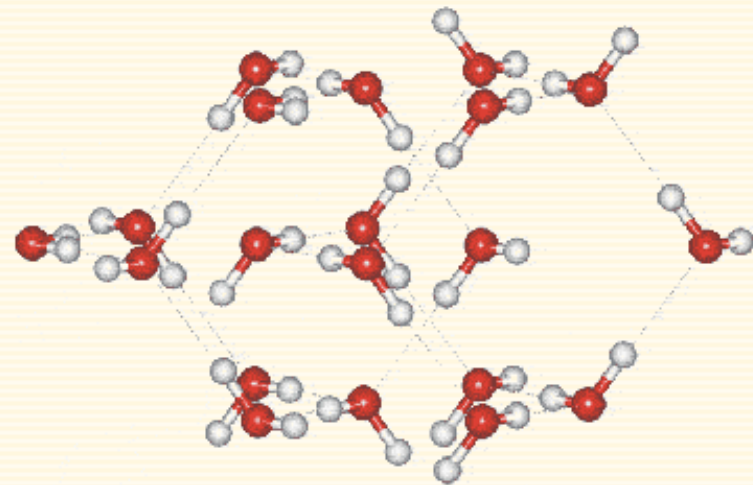




Ice-seven (Ice VII) and Ice-ten (Ice X)

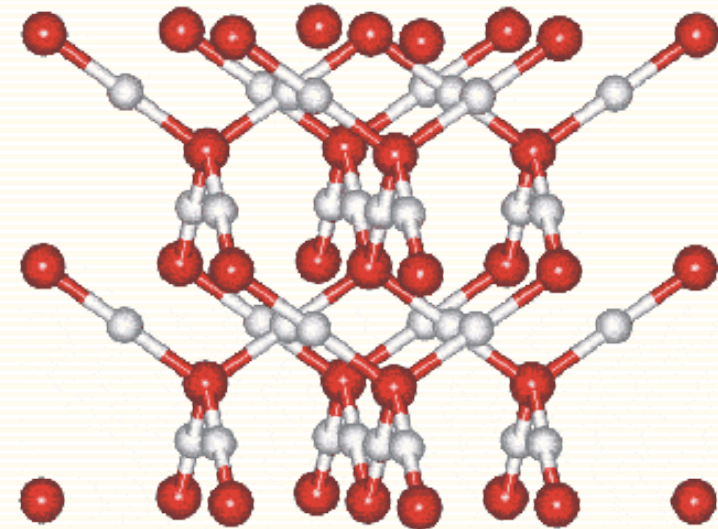
Ice-seven (ice VII) is formed from liquid water above 3 GPa by lowering its temperature to ambient temperatures (see [Phase Diagram](#)). It can be obtained at low temperature and ambient pressure by decompressing (D₂O) [ice-six](#) below 95 K and is metastable over a wide range of pressure, transforming into [LDA](#) above 120 K [948].

Its unit cell, which forms cubic crystal (Pn3m, 224; Laue class symmetry m-3m). Ice VII consists of two interpenetrating [cubic ice](#) lattices with hydrogen bonds passing through the center of the water hexamers and no connecting hydrogen-bonds between lattices. It has a density of about 1.65 g cm⁻³ (at 2.5 GPa and 25°C [8]), which is less than twice the cubic ice density as the intra-network O...O distances are 8% longer (at 0.1 MPa) to allow for the interpenetration. The cubic crystal (shown opposite) has cell dimensions 3.3501 Å (a, b, c, 90°, 90°, 90°; D₂O, at 2.6 GPa and 22°C [361]) and contains two water molecules.



Ice-ten

As the pressure is raised and the O...O distance contracts, ice-seven appears to undergo a continuous transition into cubic ice-ten (ice X) (still $Pn3m$ space group, $a, b, c = 2.78 \text{ \AA}$ at 62 GPa, 300 K [719]) where the ice protons are equispaced (and equally bonded) between the oxygen atoms [391] in a molecular crystal. The oxygen atoms are arranged in a body-centered cubic arrangement (8 neighbors) and the hydrogen atoms in a body-centered truncated cubic arrangement (12 neighbors). The melting curve for ice-ten has been proposed at high temperatures (1000-2400 K) [612].

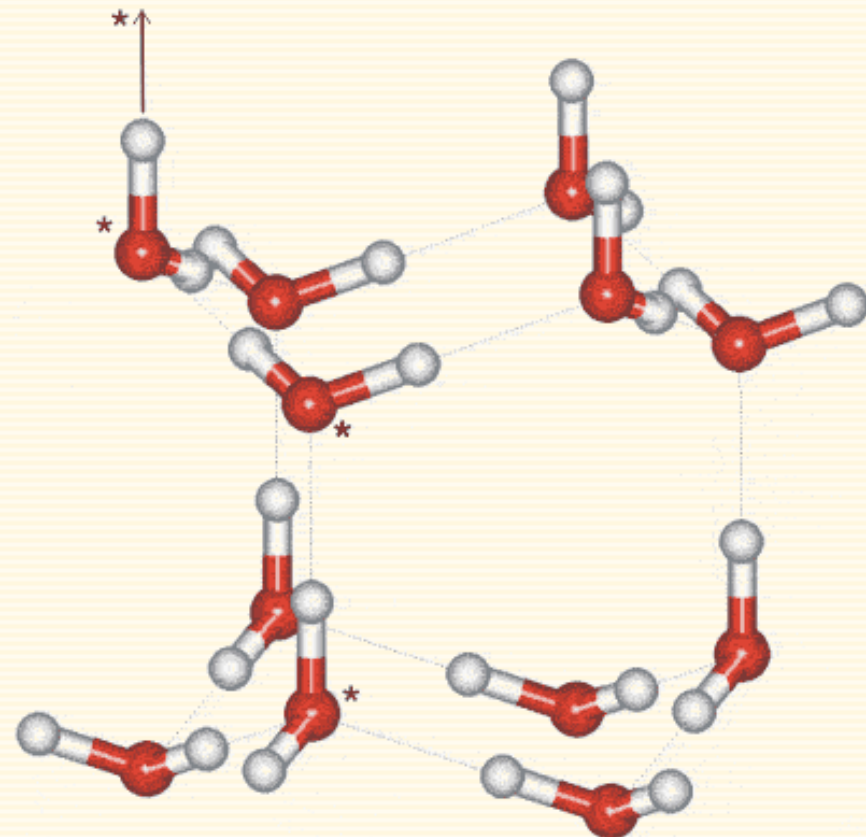


Hexagonal Ice (Ice Ih)

Hexagonal ice (ice Ih) is the form of all natural snow and ice on Earth (see [Phase Diagram](#)), as evidenced in the six-fold symmetry in ice crystals grown from water vapor (*i.e.* [snow flakes](#)).

Hexagonal ice (Space group $P6_3/mmc$, **194**;

Laue class symmetry $6/mmm$; analogous to β -tridymite silica) possesses a fairly open low-density structure, where the packing efficiency is low ($\sim 1/3$) compared with simple cubic ($\sim 1/2$) or face centered cubic ($\sim 3/4$) structures¹ (and in contrast to face centered cubic close packed solid hydrogen sulfide). The crystals may be thought of as consisting of sheets lying on top of each other. The **basic structure** consists of a hexameric box where planes consist of chair-form hexamers (the two horizontal planes, opposite) or boat-form hexamers (the three vertical planes, opposite). In this diagram the hydrogen bonding is shown ordered whereas in reality it is random.² The water molecules have a staggered arrangement of hydrogen bonding with respect to three of their neighbors, in the plane of the chair-form hexamers. The fourth neighbor (shown as vertical links opposite) has an eclipsed arrangement of hydrogen bonding.



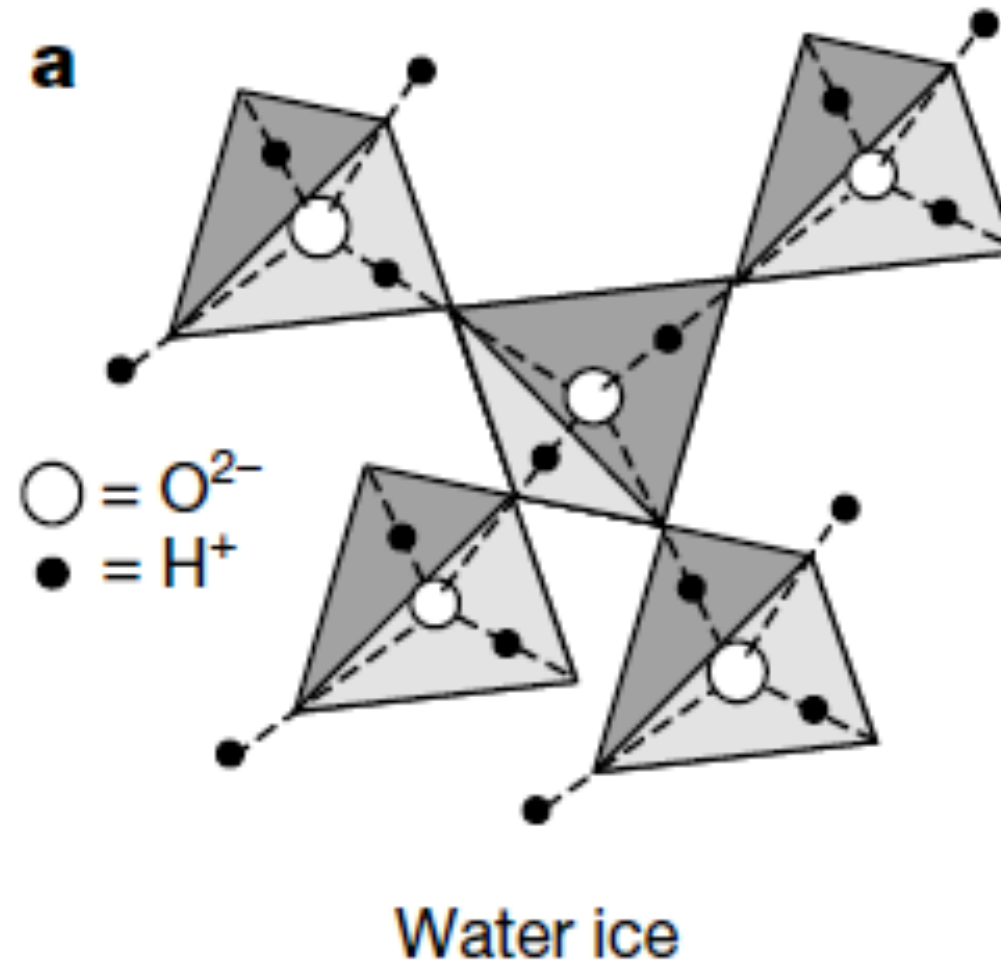


Figure 1 Schematic representation of frustration in water ice and spin ice. **a**, In water ice, each hydrogen ion is close to one or the other of its two oxygen neighbours, and each oxygen must have two hydrogen ions closer to it than to its neighbouring oxygen ions. **b**, In

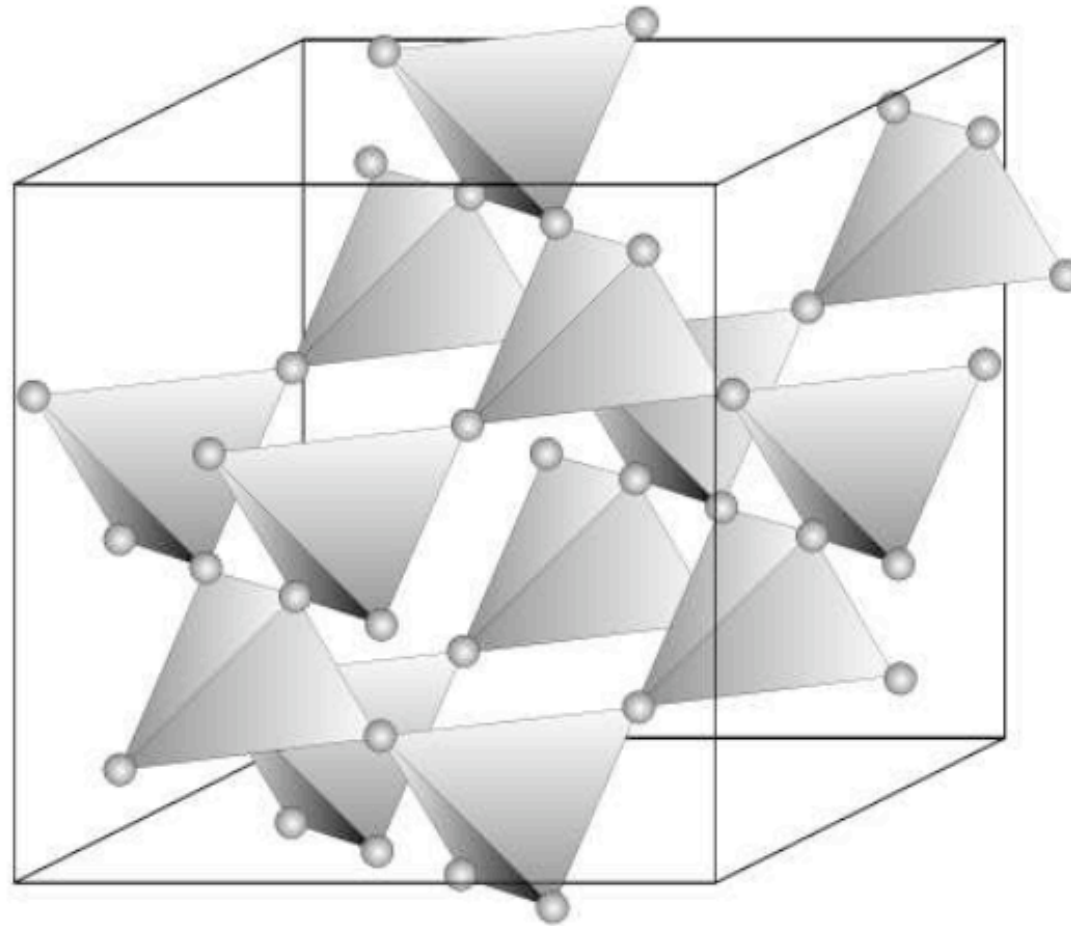


Fig.1 Pyrochlore lattice

This lattice consists of corner-shared tetrahedron. Atoms reside on the vertices of each tetrahedron.

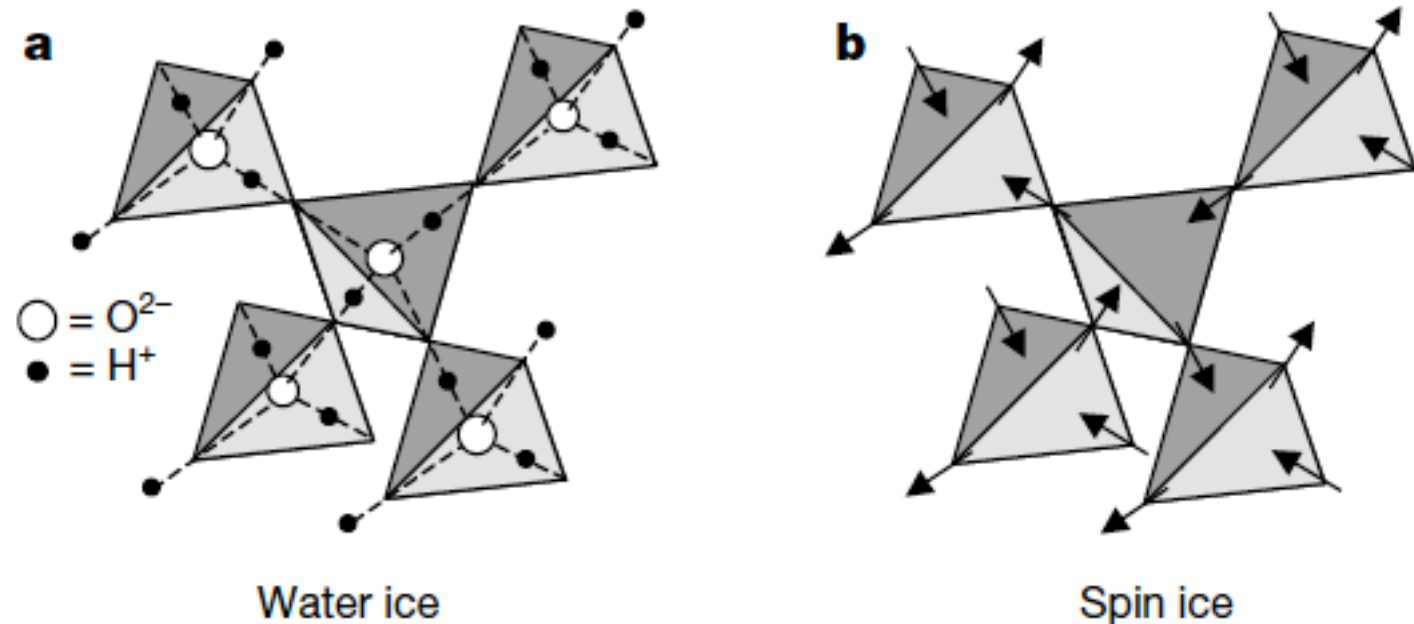
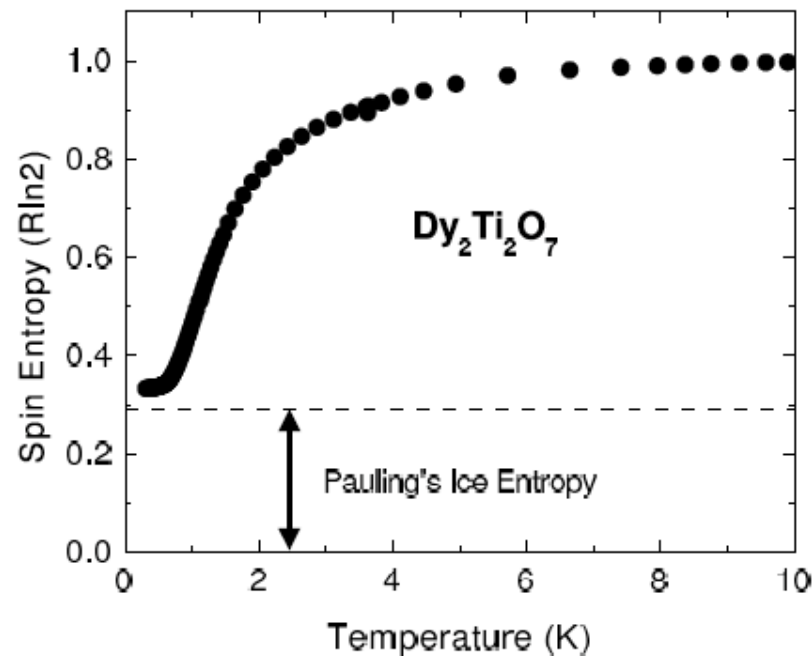


Figure 1 Schematic representation of frustration in water ice and spin ice. **a**, In water ice, each hydrogen ion is close to one or the other of its two oxygen neighbours, and each oxygen must have two hydrogen ions closer to it than to its neighbouring oxygen ions. **b**, In spin ice, the spins point either directly toward or away from the centres of the tetrahedra, and each tetrahedron is constrained to have two spins pointing in and two pointing out.

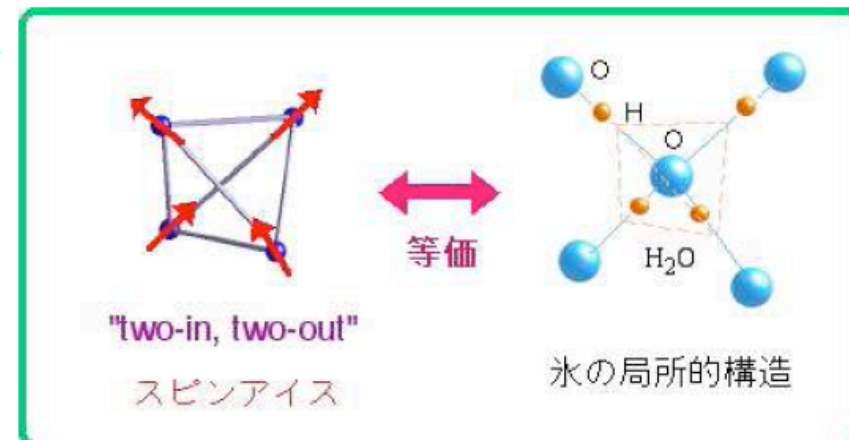
- $\text{Ho}_2\text{Ti}_2\text{O}_7$ (and $\text{Dy}_2\text{Ti}_2\text{O}_7$) are pyrochlore Ising magnets which do not order at $T \ll \Theta_W$ *Bramwell+Harris*
- Residual low- T entropy: Pauling entropy for water ice
 $\mathcal{S}_0 = (1/2) \ln(3/2)$ *Ramirez et al.*:



Spin ice and the ice rules

$$\mathcal{H} = -E \sum_i \left(\hat{\mathbf{d}}_{\kappa(i)} \cdot \mathbf{S}_i \right)^2 + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -(J/3) \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

- Spins, \mathbf{S}_i , are forced to point along local [111] axes, $\hat{\mathbf{d}}_{\kappa(i)}$
 \Rightarrow anisotropy, E , generates Ising pseudospins: $\mathbf{S}_i = \sigma_i \hat{\mathbf{d}}_{\kappa(i)}$
- there are four sublattices, κ , with $\hat{\mathbf{d}}_{\kappa} \cdot \hat{\mathbf{d}}_{\kappa'} = -1/3$
 $\Rightarrow J$ for pseudospins changes sign!
- Ground states have $\sum \sigma_i = 0$ for each tetrahedron
- These are the two-in two-out states (Bernal-Fowler ice rules)



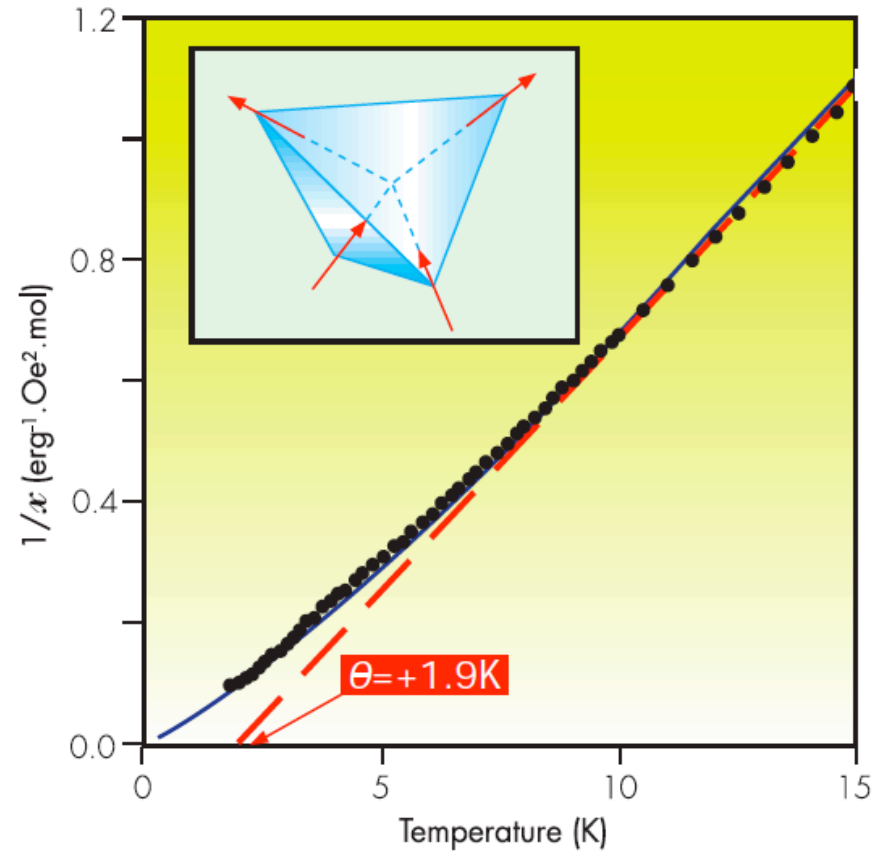


Figure F14.1. The inverse susceptibility of $\text{Ho}_2\text{Ti}_2\text{O}_7$ with a Monte Carlo simulation of the spin ice model shown as a blue line, and the standard Curie-Weiss law as a red line. The inset shows the ground state of a single tetrahedron of spins with ferromagnetic coupling and $\langle 111 \rangle$ anisotropy.

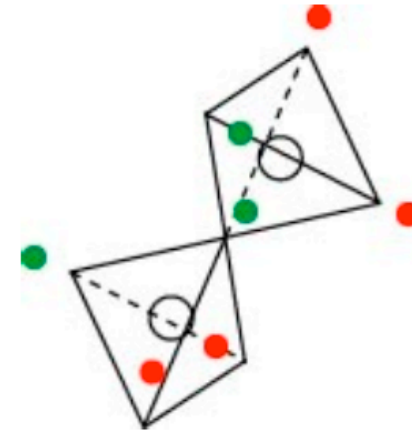
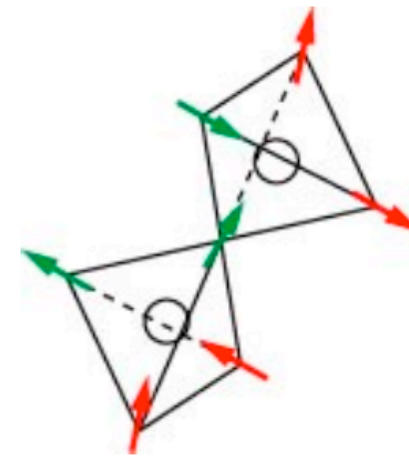


Fig.3 Proton ordering in water ice



Spin configuration in a spin ice