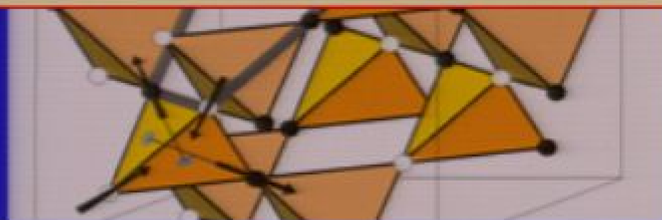
Title: Recent developments in the physics of spin ice and related quantum cousin

Date: May 26, 2010 04:45 PM

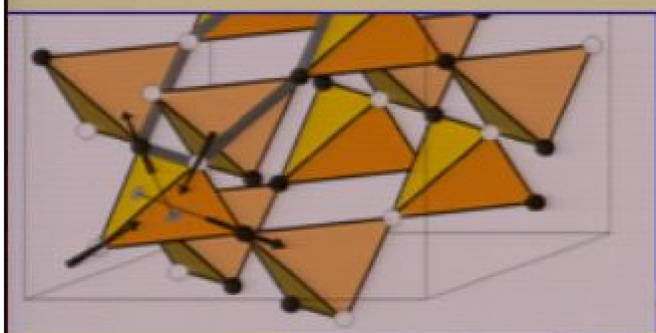
URL: http://pirsa.org/10050073

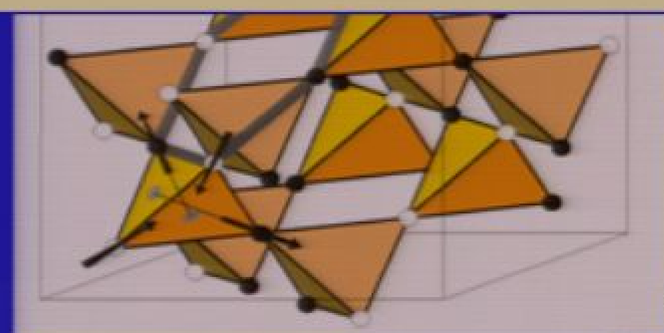
Abstract: In the Ho2Ti2O7 and Dy2Ti2O7 magnetic pyrochlore oxides, the Ho and Dy Ising magnetic moments interact via geometrically frustrated effective ferromagnetic coupling. These systems possess and extensive zero entropy related to the extensive entropy of ice water -- hence the name spin ice. The classical ground states of spin ice obey a constraint on each individual tetrahedron of interacting spins -- the so-called "ice rules". At large distance, the ice-rules can be described by an effective divergent-free field and, therefore, by an emergent classical gauge theory. In contrast, while it would appear at first sight to relate to the spin ices, the Tb2Ti2O7 material displays properties that much differ from spin ices and the behaviour of that system has largely remained unexplained for over ten years. In this talk, I will review the key features of the (Ho,Dy)2Ti2O7 spin ice materials, discuss the recent experimental results that support the emergent gauge theory description of spin ices and discuss how Tb2Ti2O7 is perhaps a "quantum melted" spin ice.

CIfAR Quantum Materials Meeting
Montreal, May 5-8 2010



Recent Developments in Spin Ice





Michel Gingras
Department of Physics & Astronomy, University of Waterloo
&
Canadian Institute for Advanced Research/Quantum Materials Program

Scope (I)

VOLUME 91, NUMBER 16 PHYSICAL REVIEW LETTERS week ending 17 OCTOBER 2003

Coulomb and Liquid Dimer Models in Three Dimensions

David A. Huse,[1] Werner Krauth,[2] R. Moessner,[3] and S. L. Sondhi[1]

PHYSICAL REVIEW B **69**, 064404 (2004)

Pyrochlore photons: The $U(1)$ spin liquid in a $S=\frac{1}{2}$ three-dimensional frustrated magnet

Michael Hermele,[1] Matthew P. A. Fisher,[2] and Leon Balents[1]

PHYSICAL REVIEW B **74**, 024302 (2006)

Ice: A strongly correlated proton system

A. H. Castro Neto,[1] P. Pujol,[2] and Eduardo Fradkin[3]

PRL **100**, 047208 (2008) PHYSICAL REVIEW LETTERS week ending 1 FEBRUARY 2008

Unusual Liquid State of Hard-Core Bosons on the Pyrochlore Lattice

Argha Banerjee,[1] Sergei V. Isakov,[2] Kedar Damle,[1] and Yong Baek Kim[2]

PRL **103**, 247001 (2009) PHYSICAL REVIEW LETTERS week ending 11 DECEMBER 2009

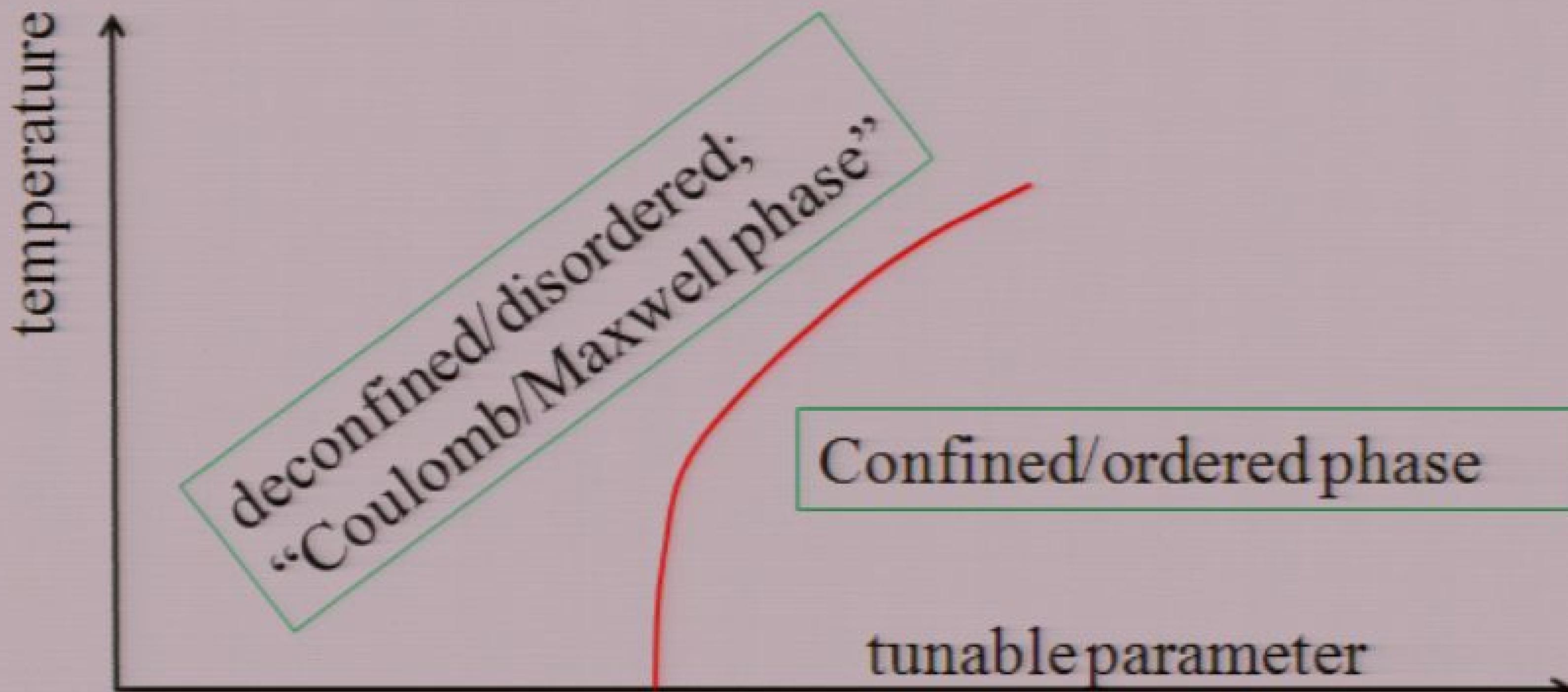
Quantum Liquid with Deconfined Fractional Excitations in Three Dimensions

Olga Sikora,[1,3] Frank Pollmann,[2] Nic Shannon,[3] Karlo Penc,[4] and Peter Fulde[1,5]

Disorder from disorder and confinement in the quantum Ising model in the pyrochlore lattice

Chyh-Hong Chern, Chen-Nan Liao, Yang-Zhi Chou; arXiv:1003.4204

Scope (II)



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Ice: A strongly correlated proton system

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$$H_{\text{eff}} = J_z \sum_{\langle i,j \rangle} S_i^z S_j^z + J_\perp \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right) \rightarrow \cdots \text{QED on lattice}$$

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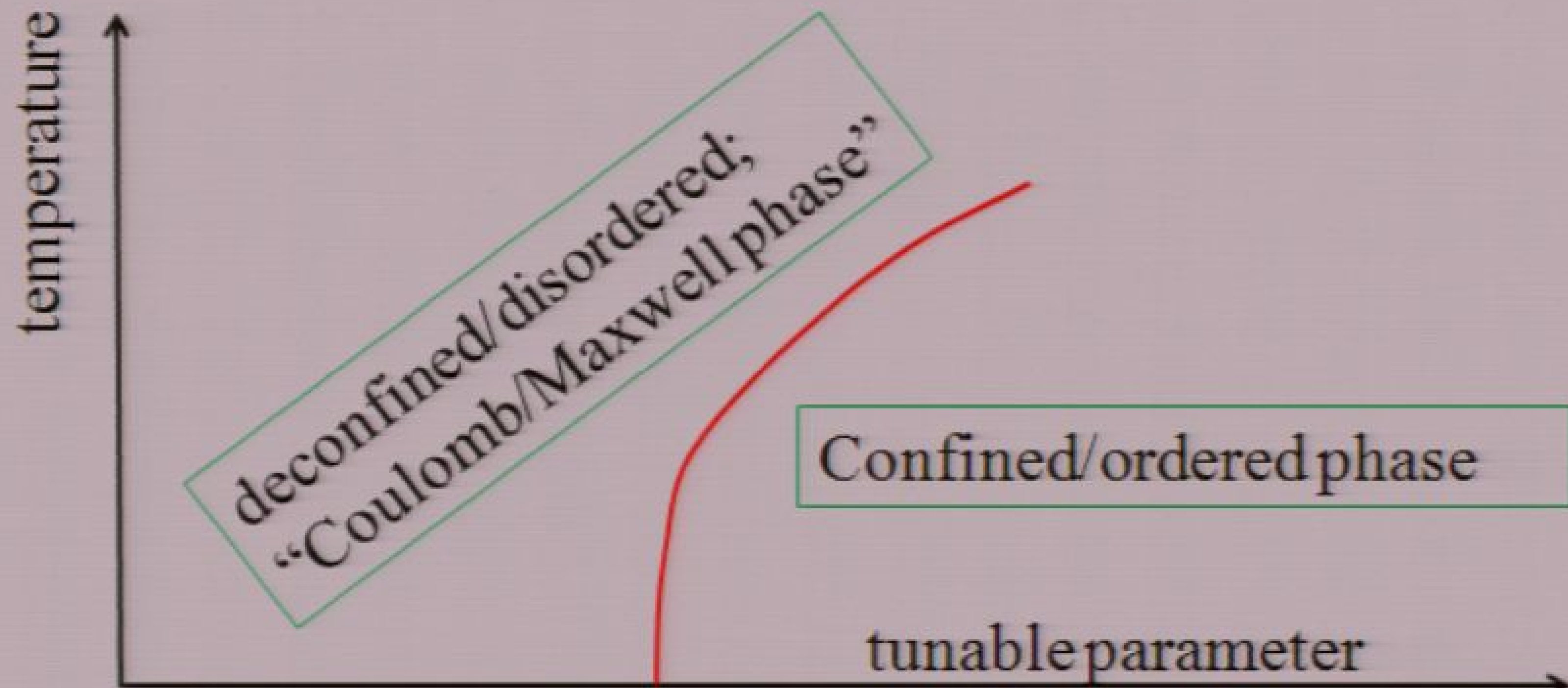

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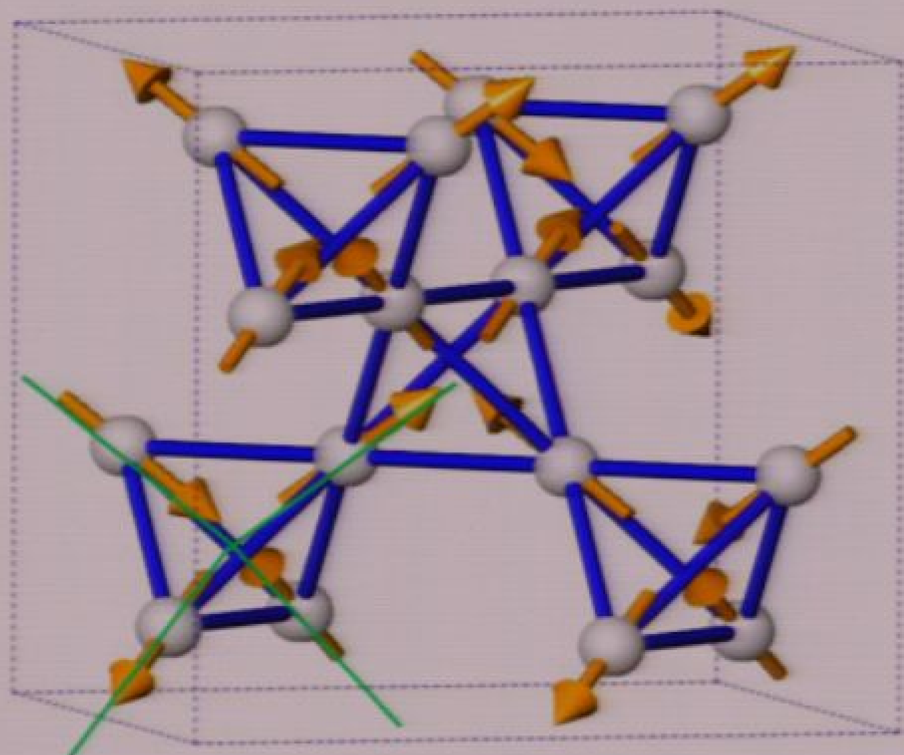
Can we find H_{eff} in a real material context?

Philosophy

- Since the theoretical work predicting a Coulomb/Maxwell phase makes use as starting point of the underlying (classical) Coulomb phase of an extensively degenerate Ising antiferromagnet on the pyrochlore lattice (pyrochlore Ising AF) …

- Can we seek a candidate material with exotic properties in the "parametric vicinity" of the materialistic equivalent of the pyrochlore Ising AF, that is the *spin ice* materials?

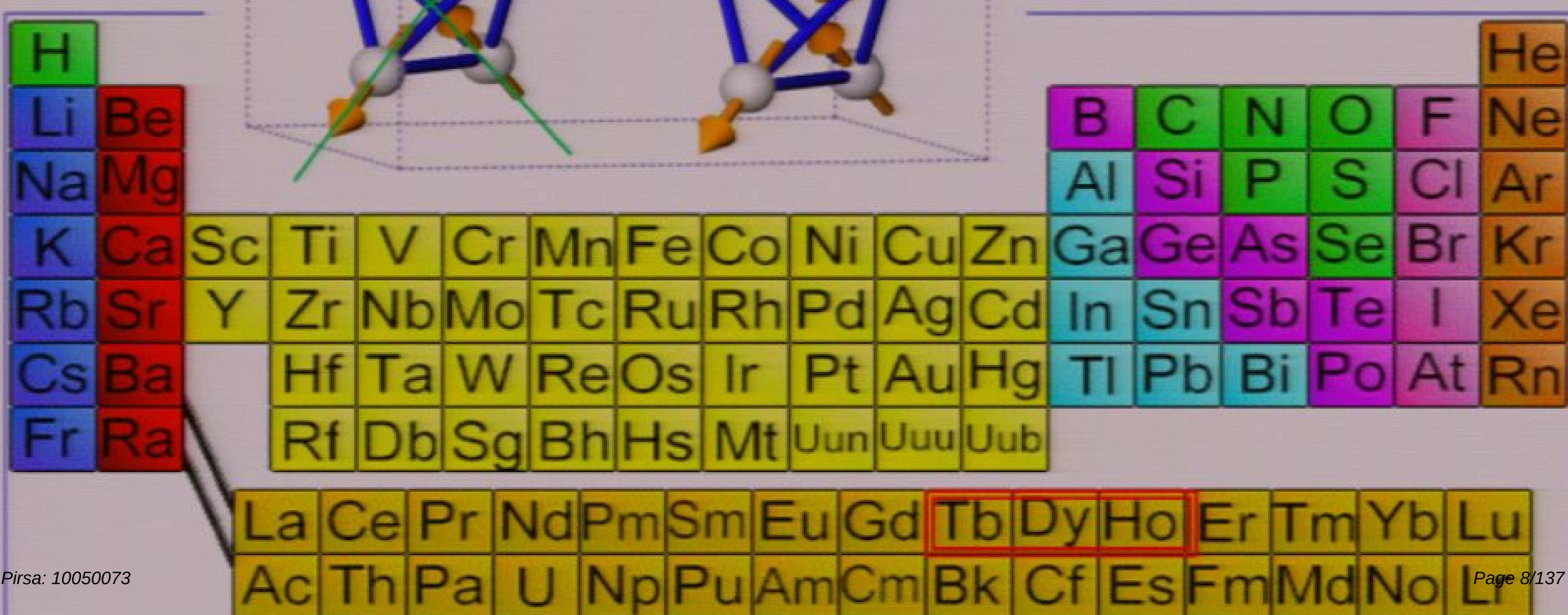
⟨111⟩ Ising pyrochlores



Ho$_2$Ti$_2$O$_7$

Dy$_2$Ti$_2$O$_7$

Tb$_2$Ti$_2$O$_7$



Collaborators

Theory

- Paul McClarty (U. Waterloo)
- Hamid Molavian (U. Waterloo)
- Taras Yavorsk'ii (U. Waterloo)

Experimental

- S. Bramwell (UCL, London)
- T. Fennell (ILL, Grenoble)

Outline

1. **Introduction – a review of spin ice physics**
   - *Frustrated ferromagnet & ice rules*
   - *extensive low-temperature entropy*
   - *role of dipolar interactions*
2. **Spin ice – recent developments**
   - *Coulomb phase and divergence free field*
   - *Spin-spin correlations*
   - *Excitations in the Coulomb phase and monopoles*
   - *Magnetic-field induced dissociation of ice rules*
3. **Spin liquid physics of $Tb_2Ti_2O_7$**
   - *Corrections to Ising model*
   - *"Quantum spin ice"*
4. **Conclusion**

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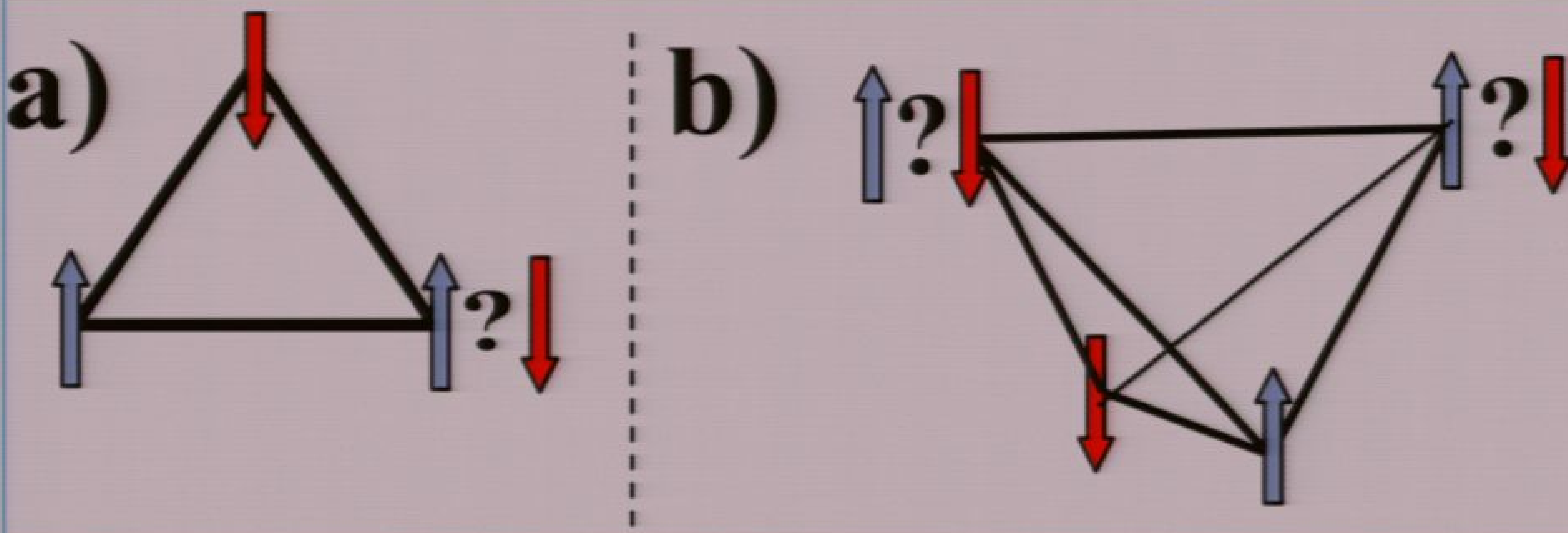
Frustration in antiferromagnets

$H_{ij} = -JS_i^z S_j^z \;;\; S_i^z = \pm 1$

$J > 0$: ferromagnetic $\rightarrow$ nonfrustrated

$J < 0$: antiferromagnetic $\rightarrow$ frustrated



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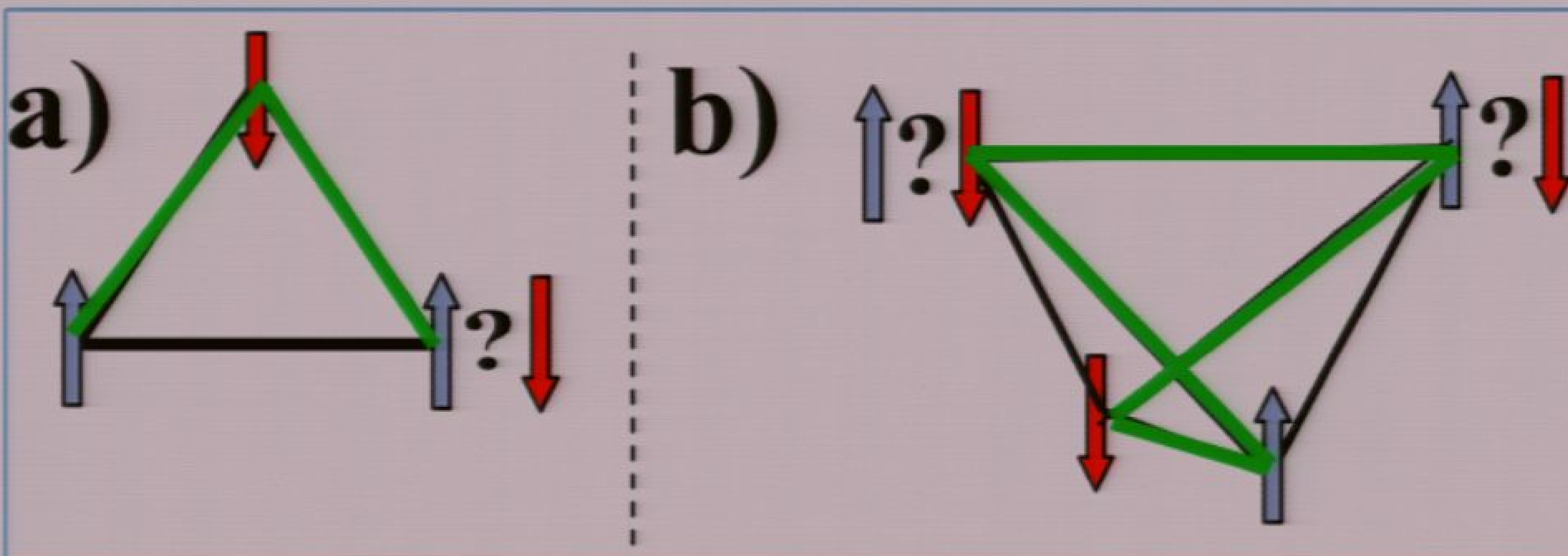
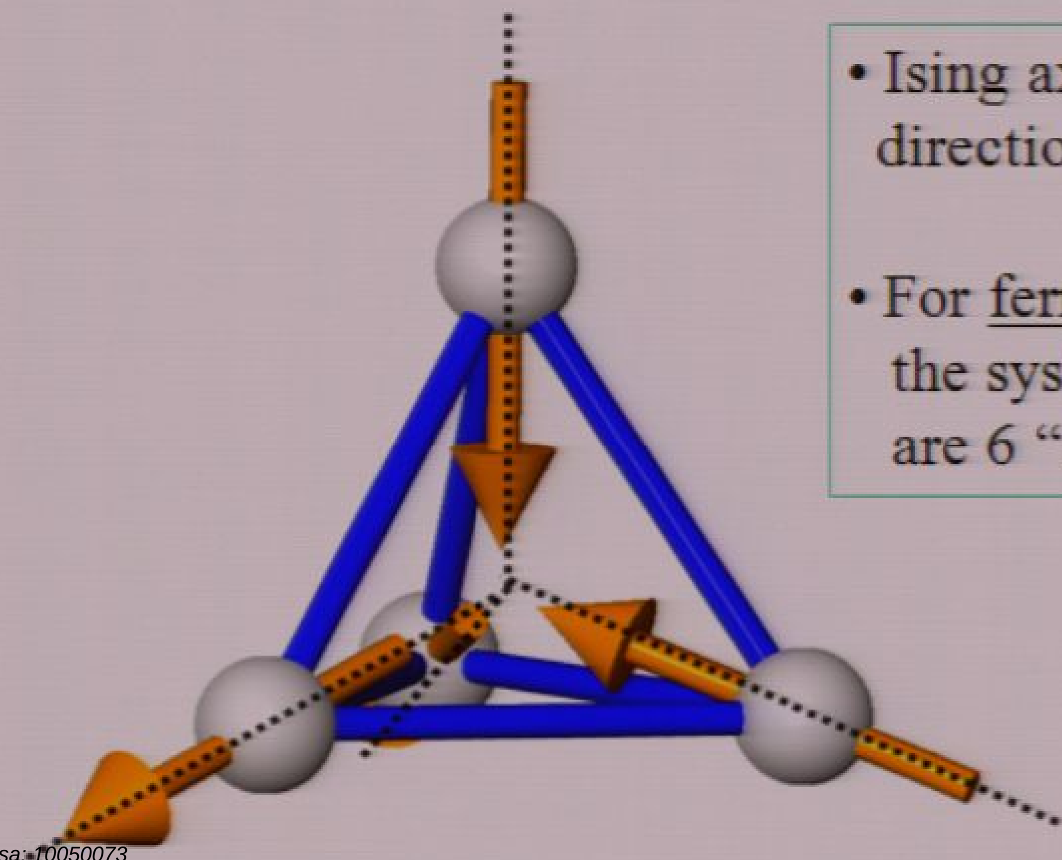


Frustrated ferromagnetism in pyrochlores with local Ising (111) anisotropy

$Ho_2Ti_2O_7$

$Dy_2Ti_2O_7$

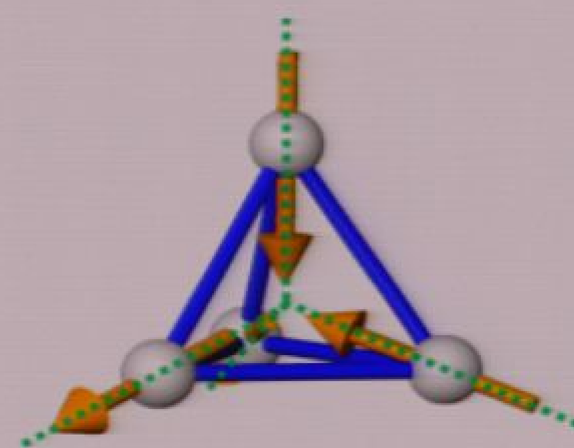
Ho^{3+}, Dy^{3+} contain Ising moments at sufficiently low temperature.



- Ising axes comprise the [111] directions of the cubic unit cell.
- For <u>ferromagnetic interactions,</u> the system is now frustrated and there are 6 "2-in/2out" spin configurations

Frustrated ferromagnetism in pyrochlores with local Ising (111) anisotropy

$$H = -J_{ex} \sum_{\langle i,j \rangle} \vec{S}_i \bullet \vec{S}_j \; ;$$



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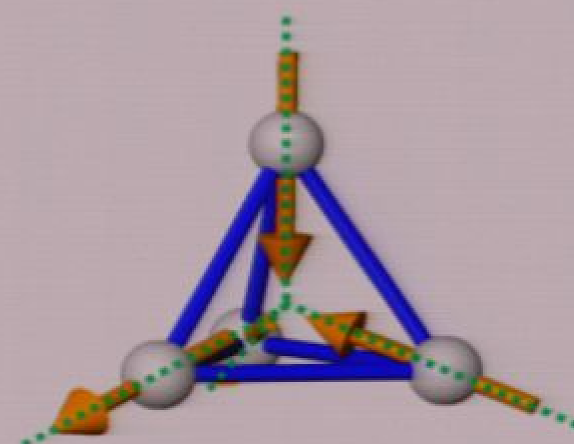

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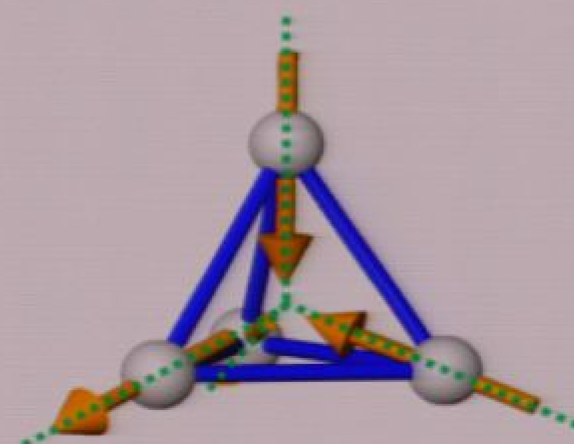

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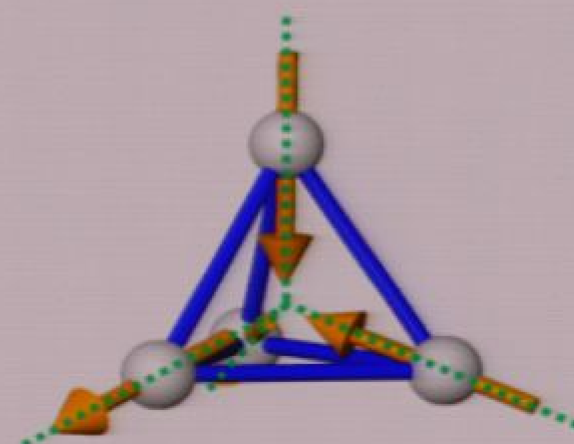
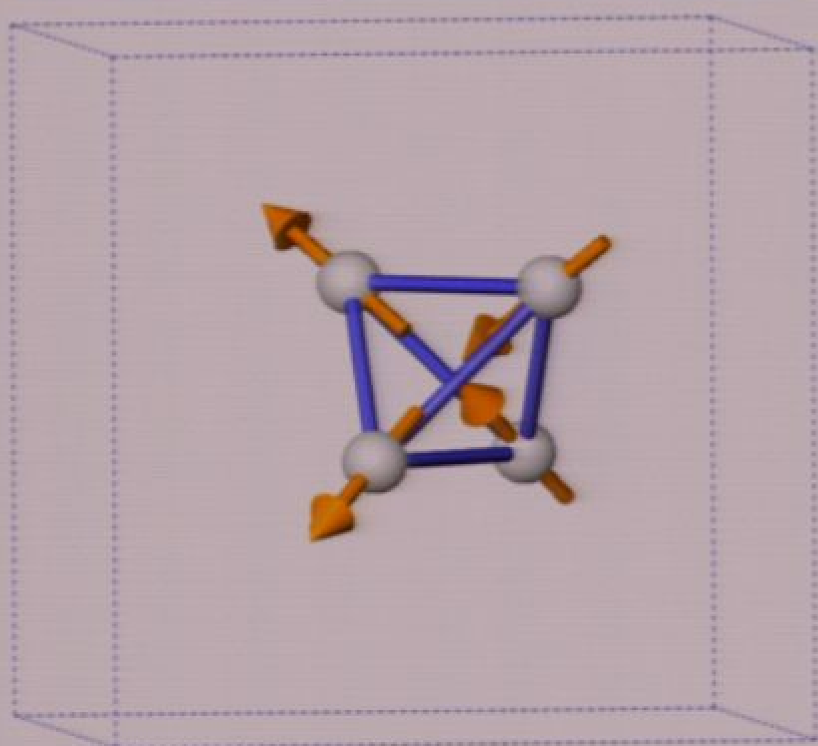
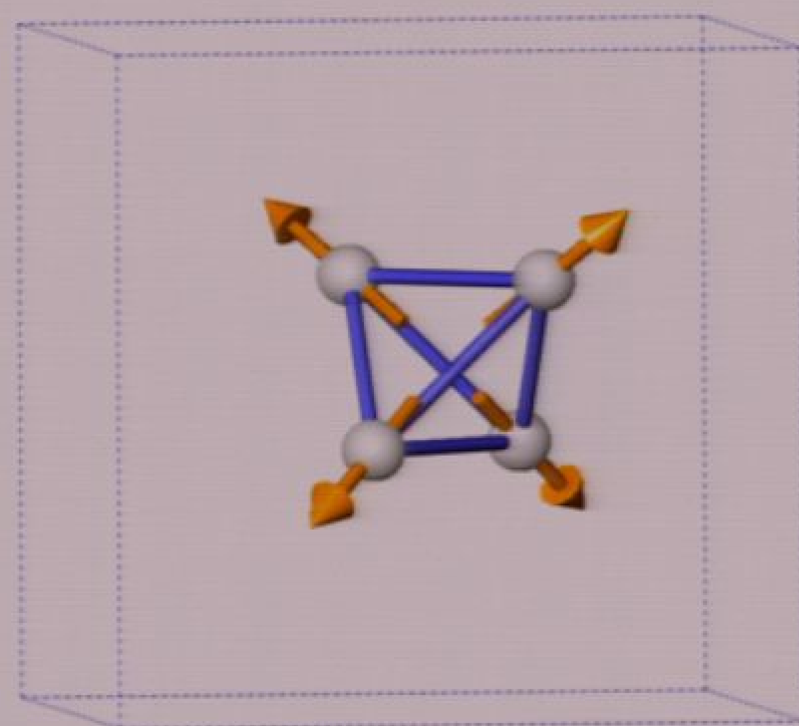


Sign swap – unfrustrated global FM has become effective frustrated Ising AF under constraint of infinite local [111] easy-axis anisotropy

- $J_{ex}>0$: ferromagnetic
- "two-in/two-out"
- **Frustrated**

- $J_{ex}<0$: antiferromagnetic
- "all-in/all-out"
- **Not frustrated**





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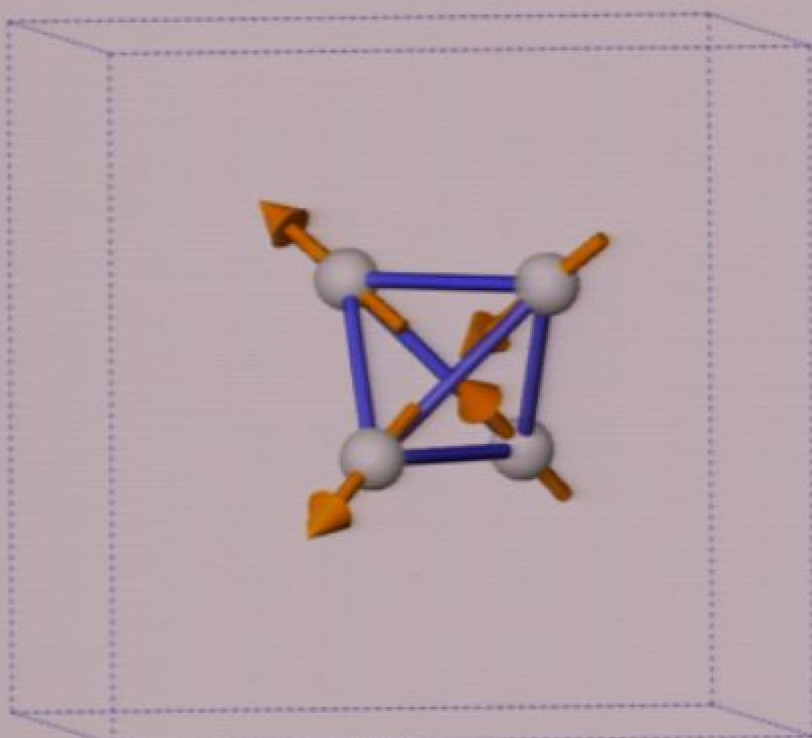
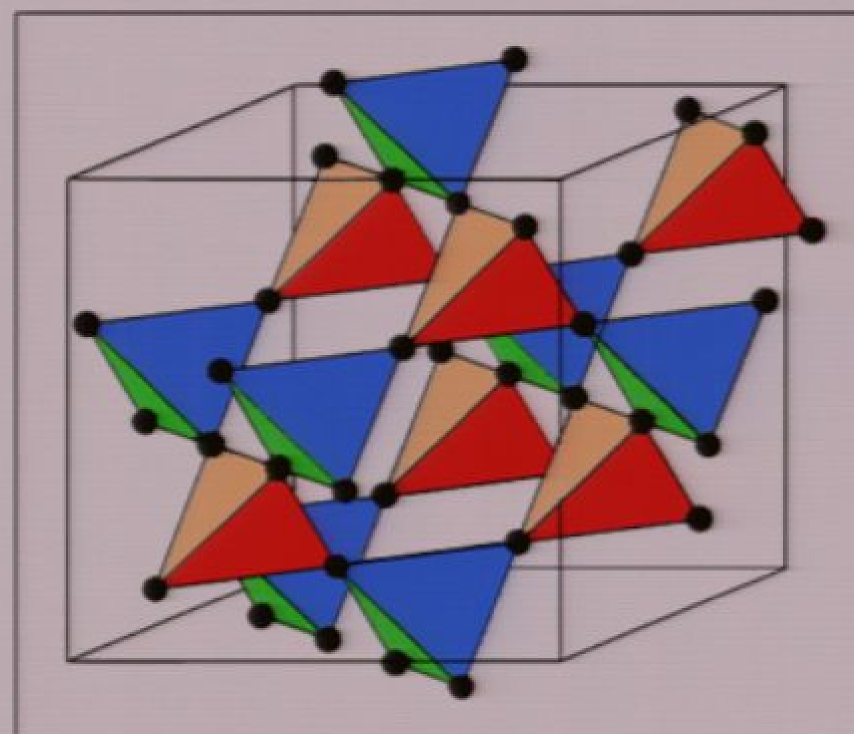
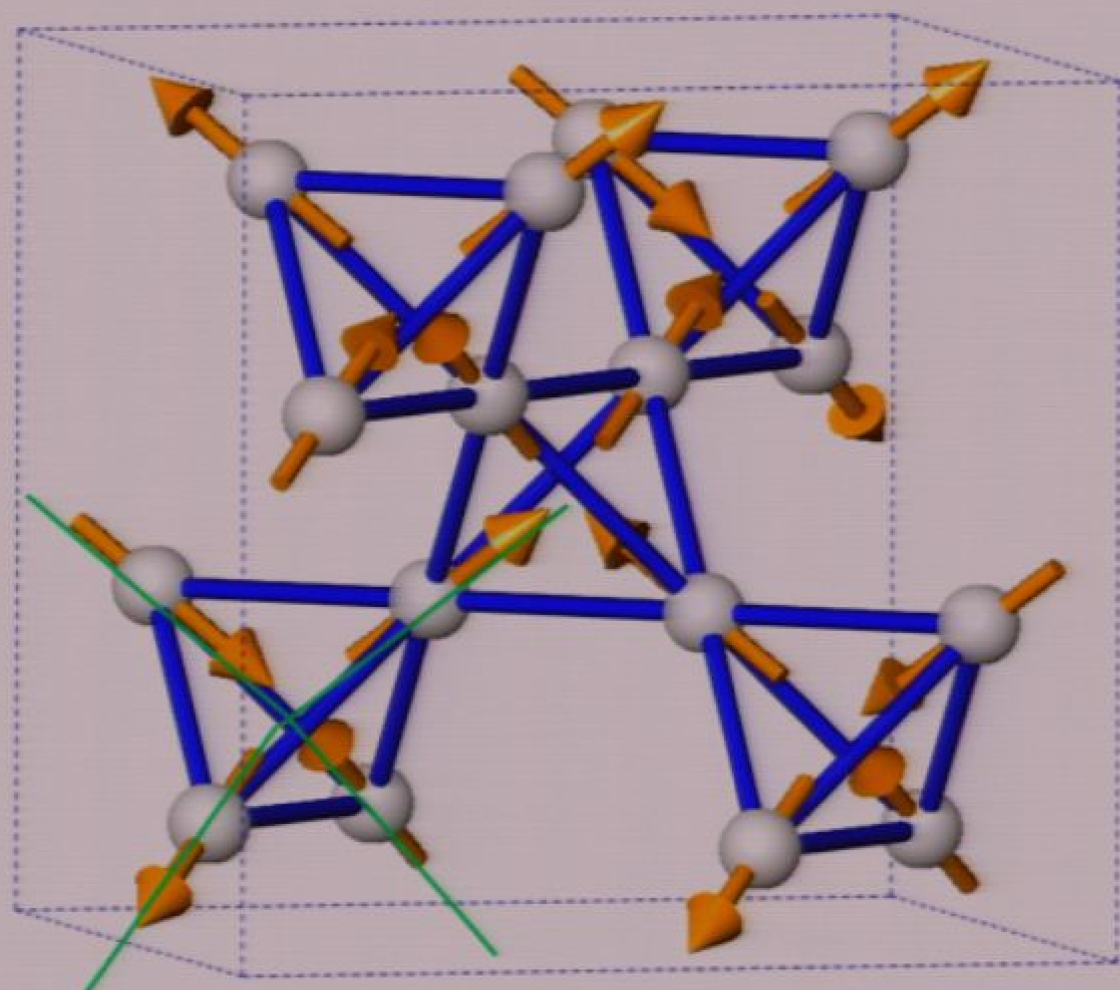




"Two-in/two-out" ice rules



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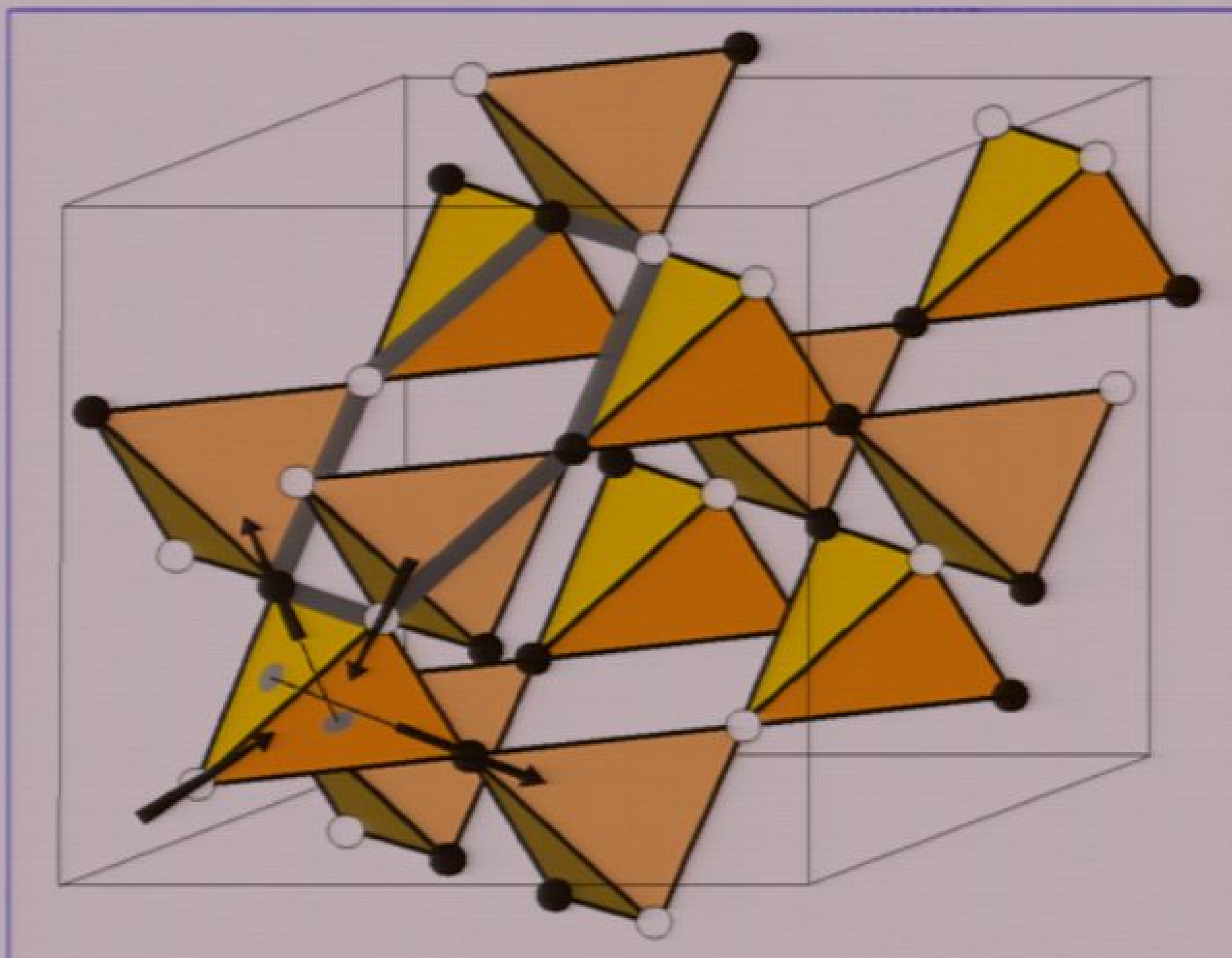

Degeneracy of Ising Pyrochlore Ferromagnet

For N moments on the pyrochlore lattice with n.n. ferromagnetic J_{ij} exchange, there are

$$\Omega \approx 6^{N/4}(6/16)^{N/4}$$

equivalent groundstates of the system!

So at T=0, the entropy per spin is $$S_{T=0} = k_B \frac{1}{2} \ln \frac{3}{2}$$

Same (Pauling) entropy at T=0 as ice water!!!
hence the name "spin ice"

M. J. Harris, S. T. Bramwell, D. F. McMorrow, T. Zeiske and K. W. Godfrey *Phys. Rev. Lett.* 79, 2554 (1997)

Proton Position in Ice vs Spin Orientation in Pyrochlore

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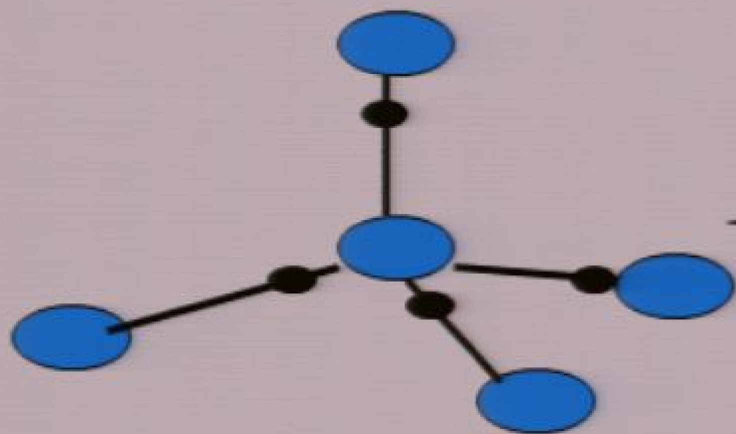
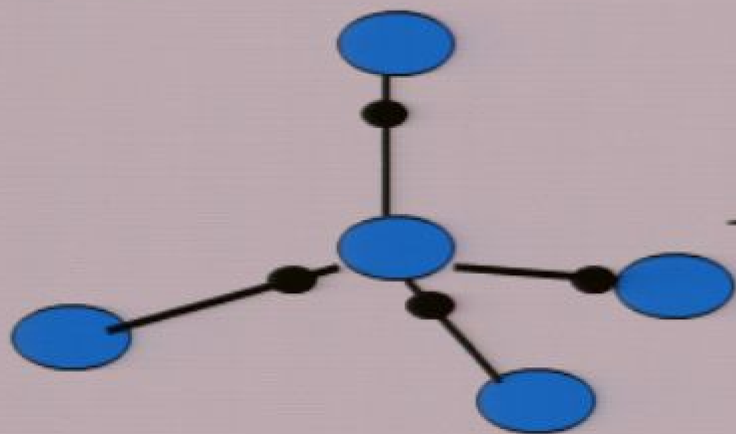


- Tetrahedral proton coordination
- Bernal-Fowler ice rules: "*two protons near/two protons far*"

Proton Position in Ice vs Spin Orientation in Pyrochlore



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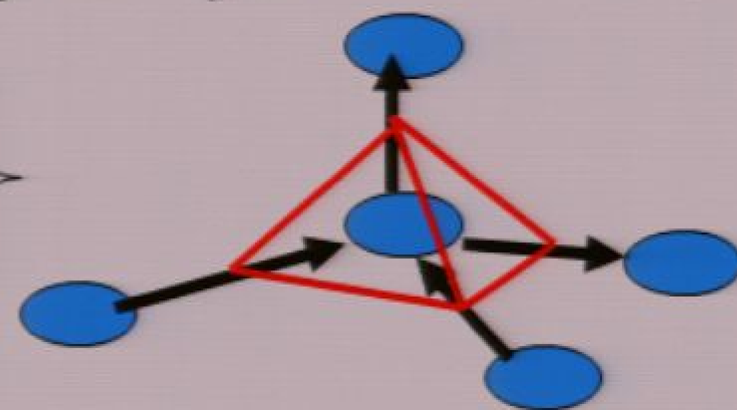
roton displacement: vector at mid-point



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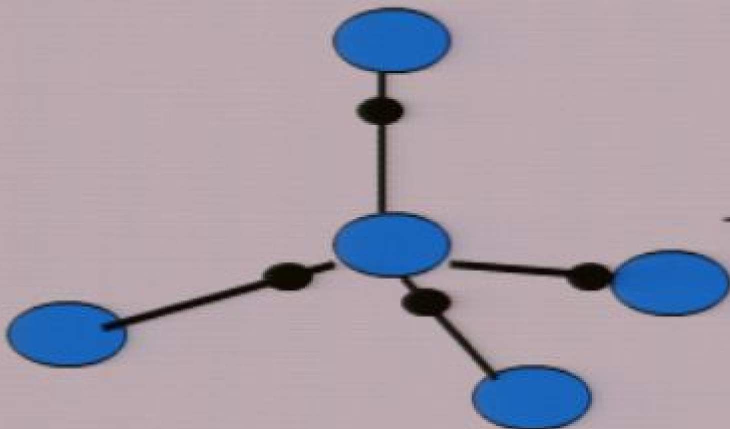

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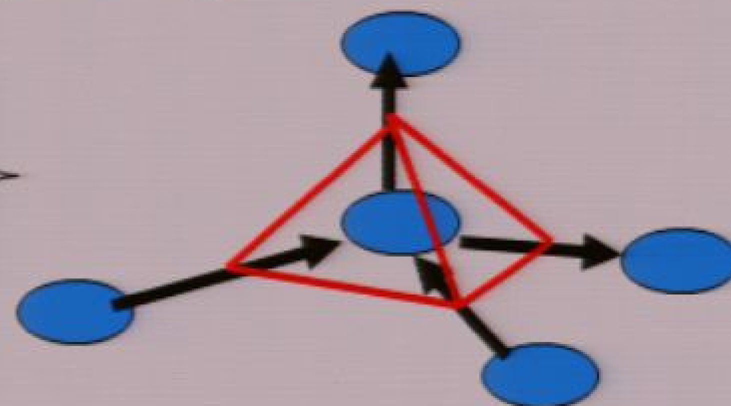
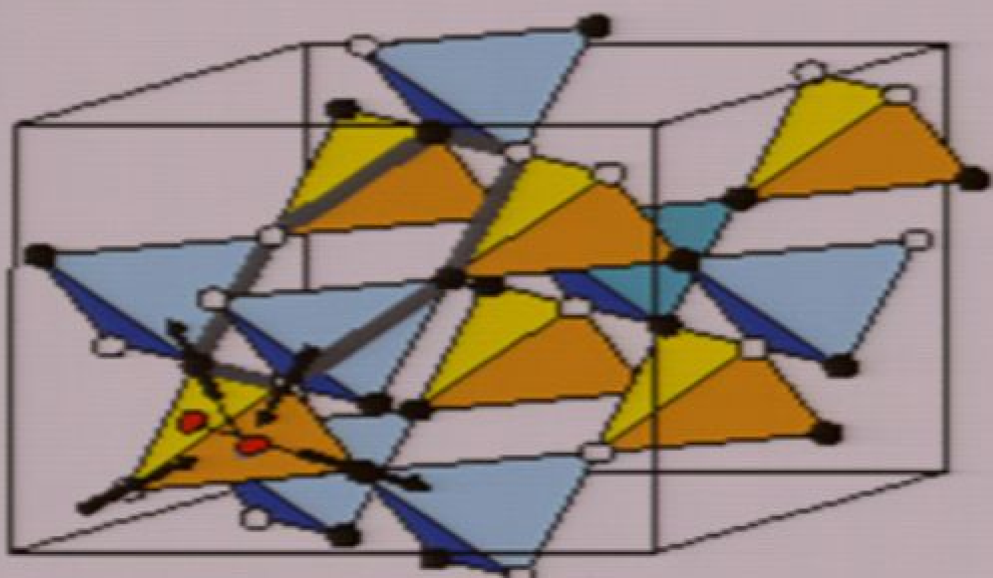
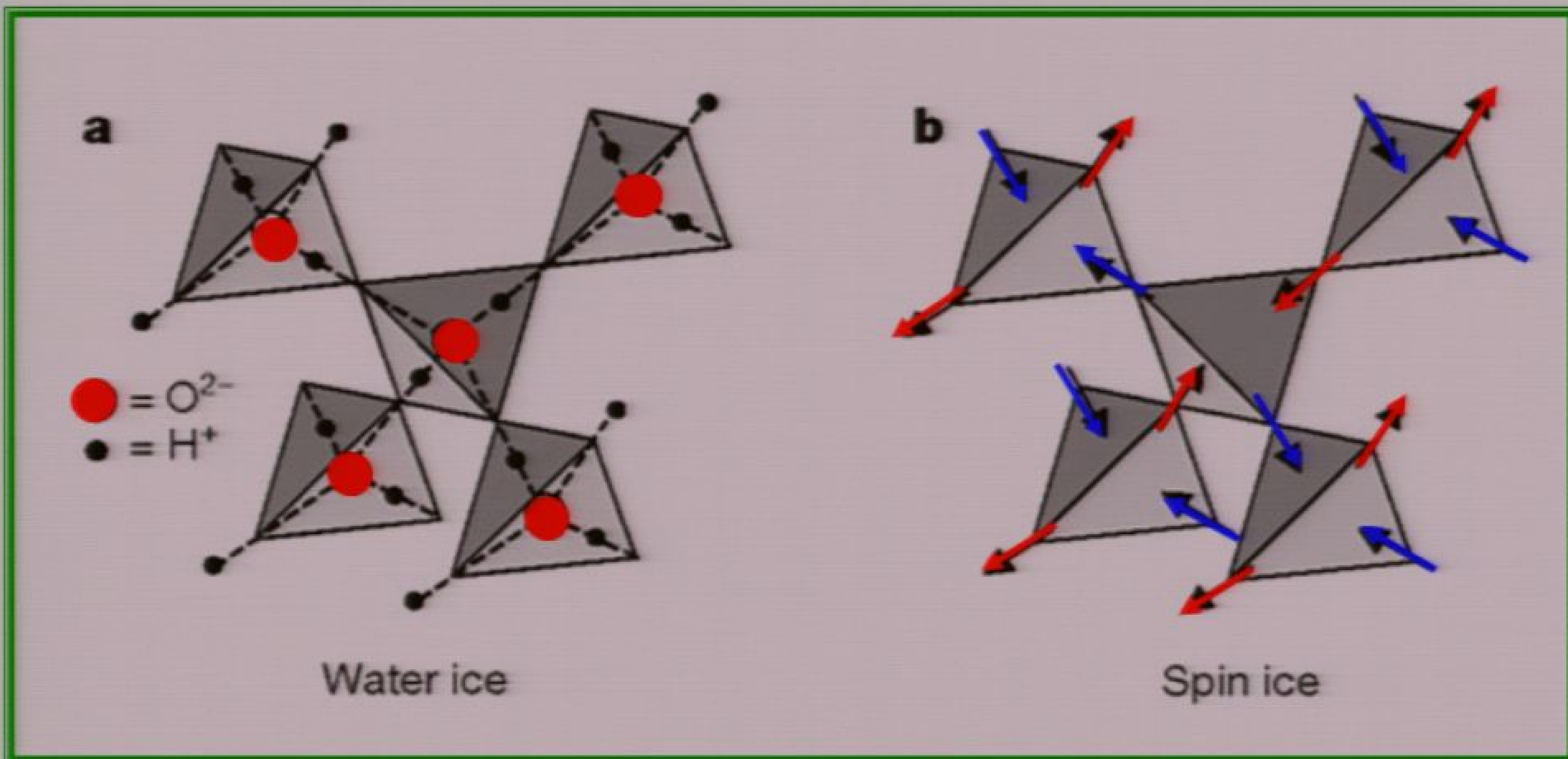


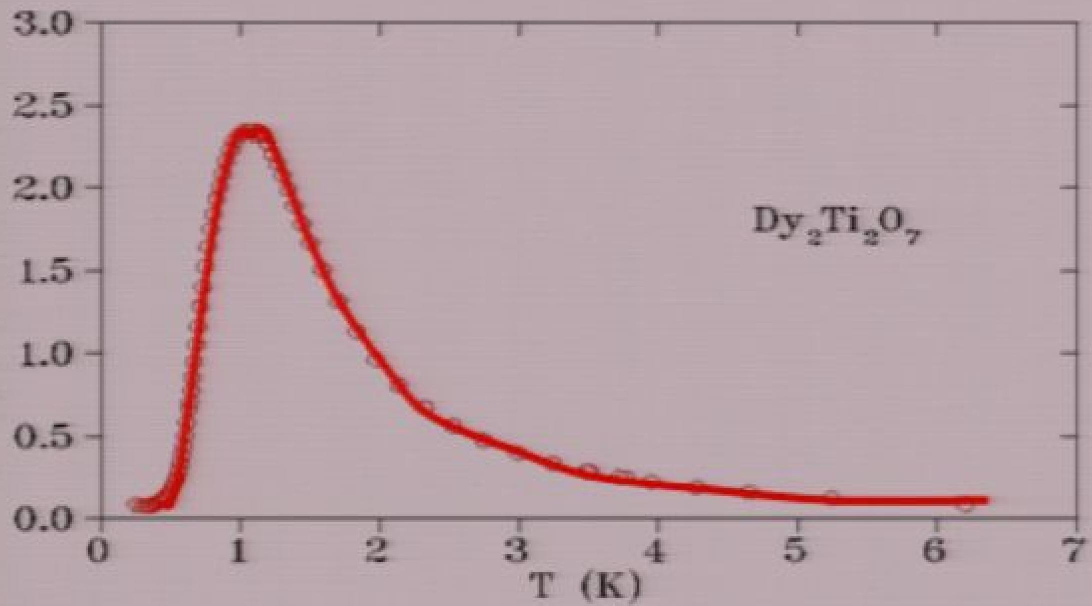


Magnetic moments on pyrochlore lattice

S. T. Bramwell and M. J. Harris,
J. Phys. Condens. Matter 10, L215 (1998)


a
= O2−
= H+
Water ice
b
Spin ice

Real materials show manifestations of Pauling's ground state entropy magnetic analogues of water ice



Ramirez *et. al*, "*Zero Point Entropy in Spin Ice*", Nature **399**, 333 (1999)

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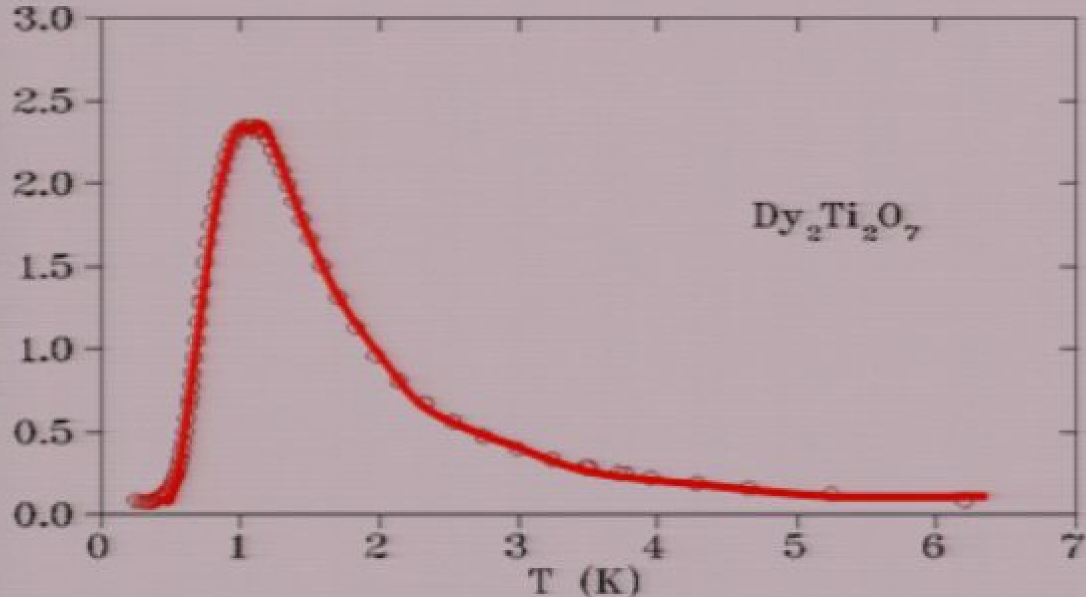

$$S(T_2) - S(T_1) = \int_{T_1}^{T_2} \frac{C(T)}{T} dT$$

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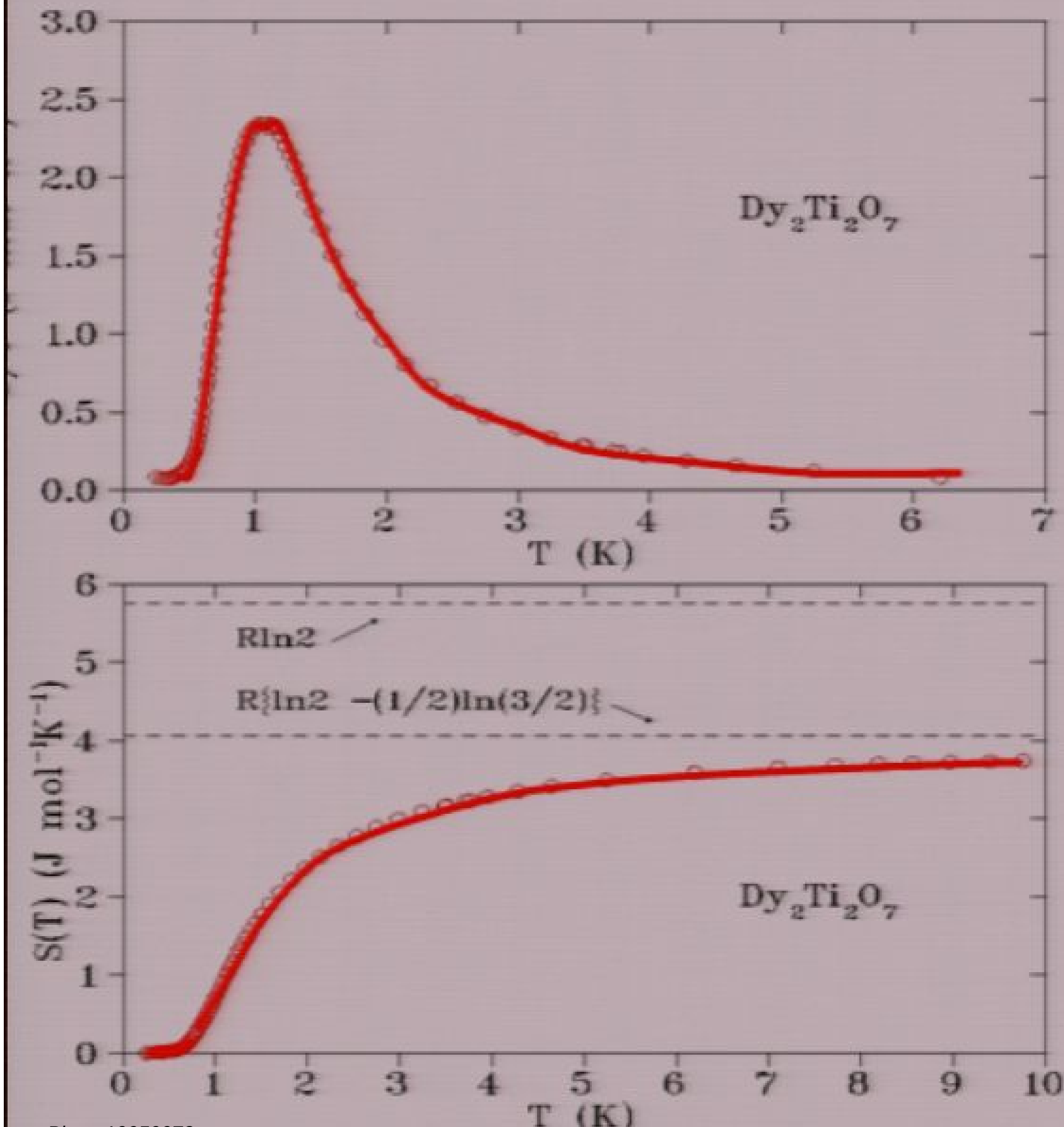

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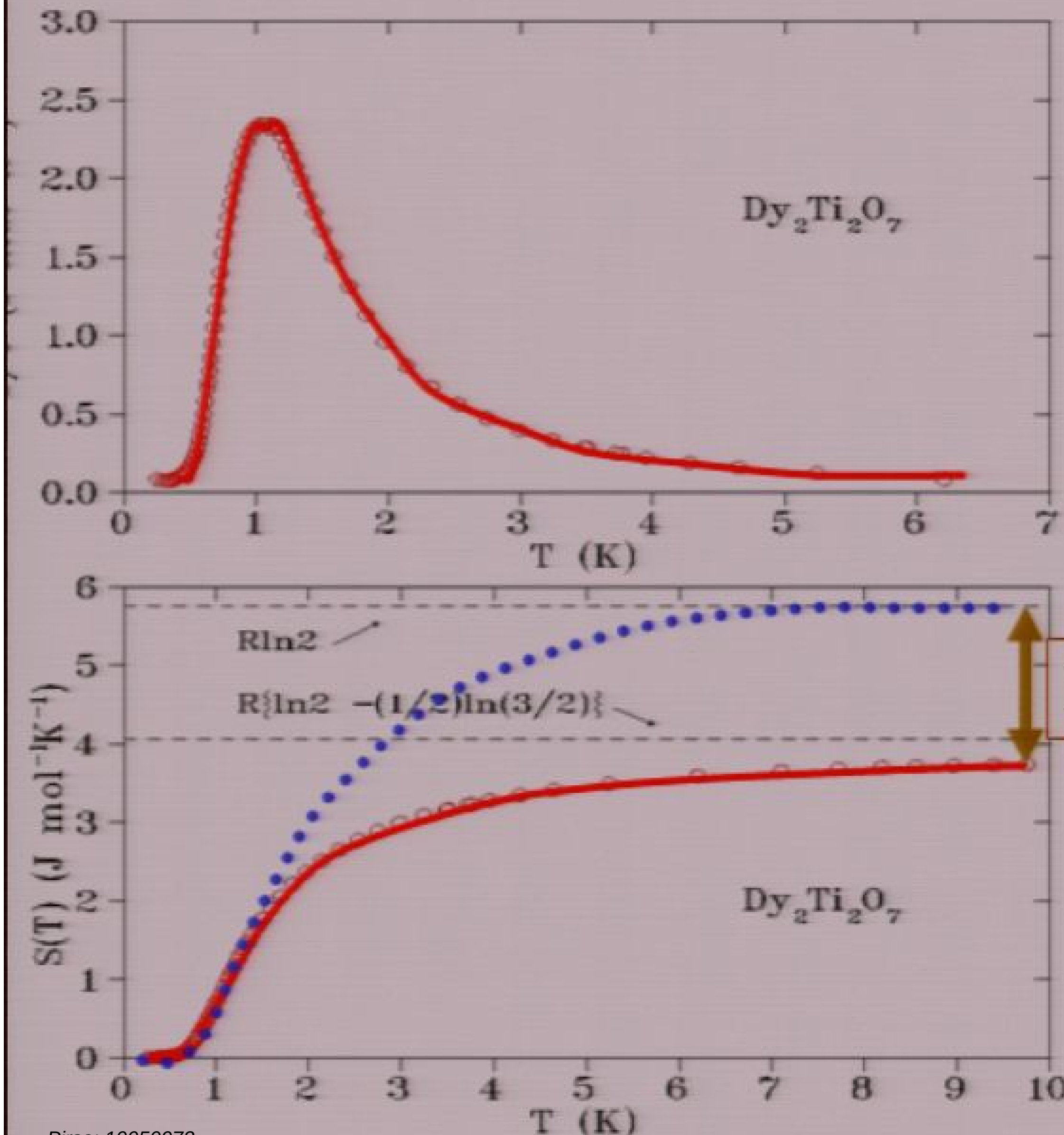

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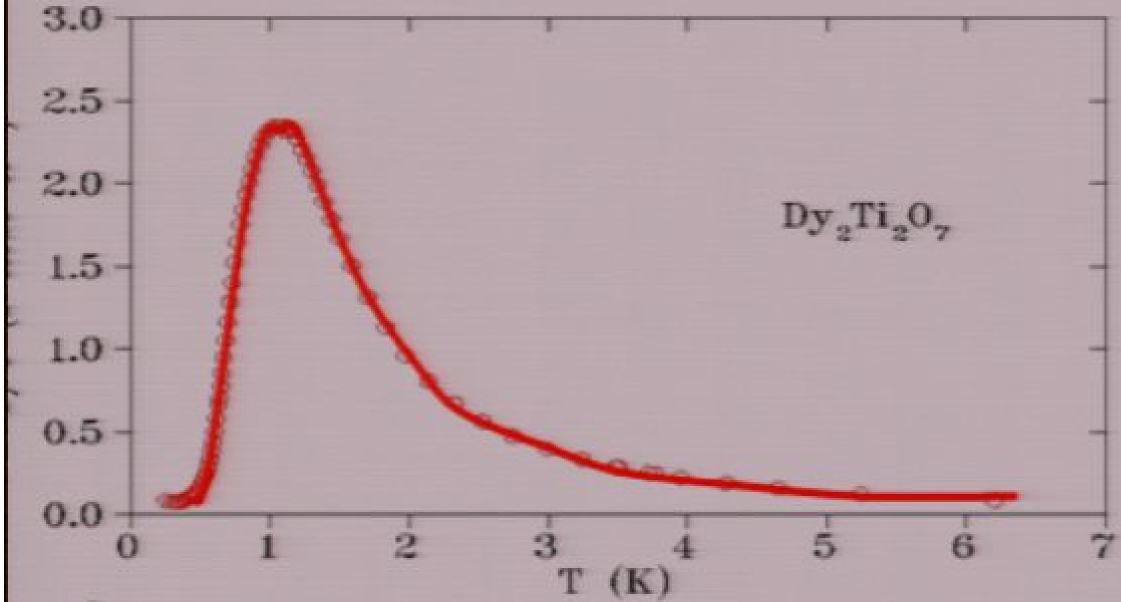

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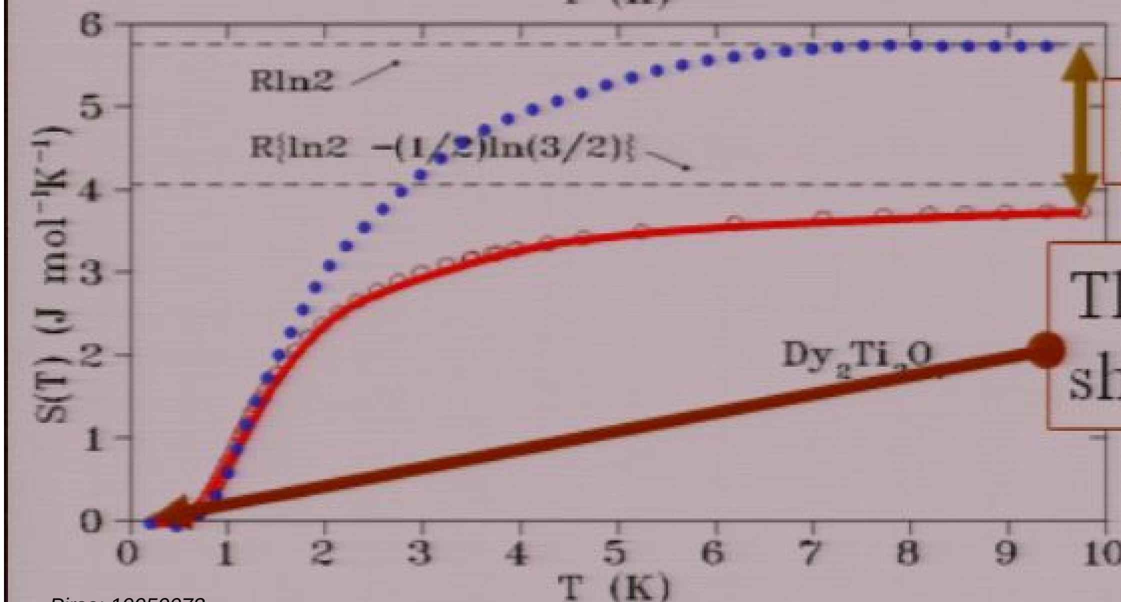

Difference is Pauling's S_0 !!

This means, the value of $S(T=0)$ should have beeen set to S_0 not 0

Ramirez *et. al*, "*Zero Point Entropy in Spin Ice*", Nature **399**, 333 (1999)

Hamiltonian / Standard Dipolar Spin Ice Model (s-DSM)

$$H = -J_1 \sum_{\langle i,j \rangle} \left(\hat{z}_i \bullet \hat{z}_j\right) \sigma_i^z \sigma_j^z \quad ; \quad \sigma_i^z = \pm 1, \; \left(\hat{z}_i \bullet \hat{z}_j\right) = -1/3$$

Not known

$$+ D \sum_{j>i} \frac{\hat{z}_i \bullet \hat{z}_j}{\left|\vec{r}_{ij}\right|^3 / r_{nn}{}^3} - 3 \frac{(\hat{z}_i \bullet \vec{r}_{ij})(\vec{r}_{ij} \bullet \hat{z}_j)}{\left|\vec{r}_{ij}\right|^5 / r_{nn}{}^5} \sigma_i^z \sigma_j^z$$

Known

$$D = \frac{\mu_0 g^2 \mu_B^2 \langle \mathrm{J} \rangle^2}{4\pi R_{nn}^3}$$

As long as D is sufficiently large compared to J, the model gives "spin ice physics" and explains semi-quantitatively quite well equilibrium phenomena and bulk thermodynamic quantities of spin ice materials (Bramwell and Gingras, Science **294**, 1495 [2001])

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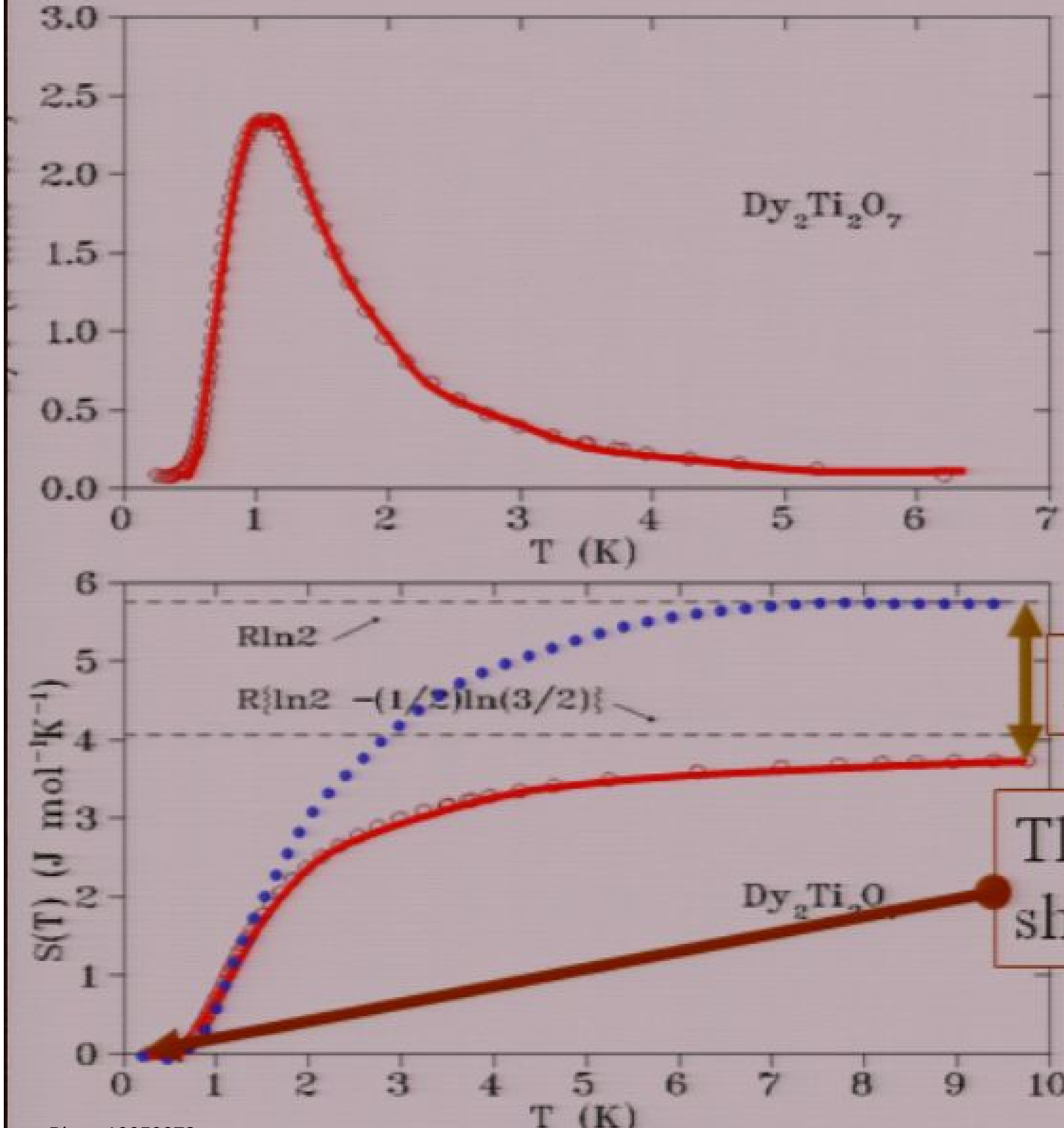

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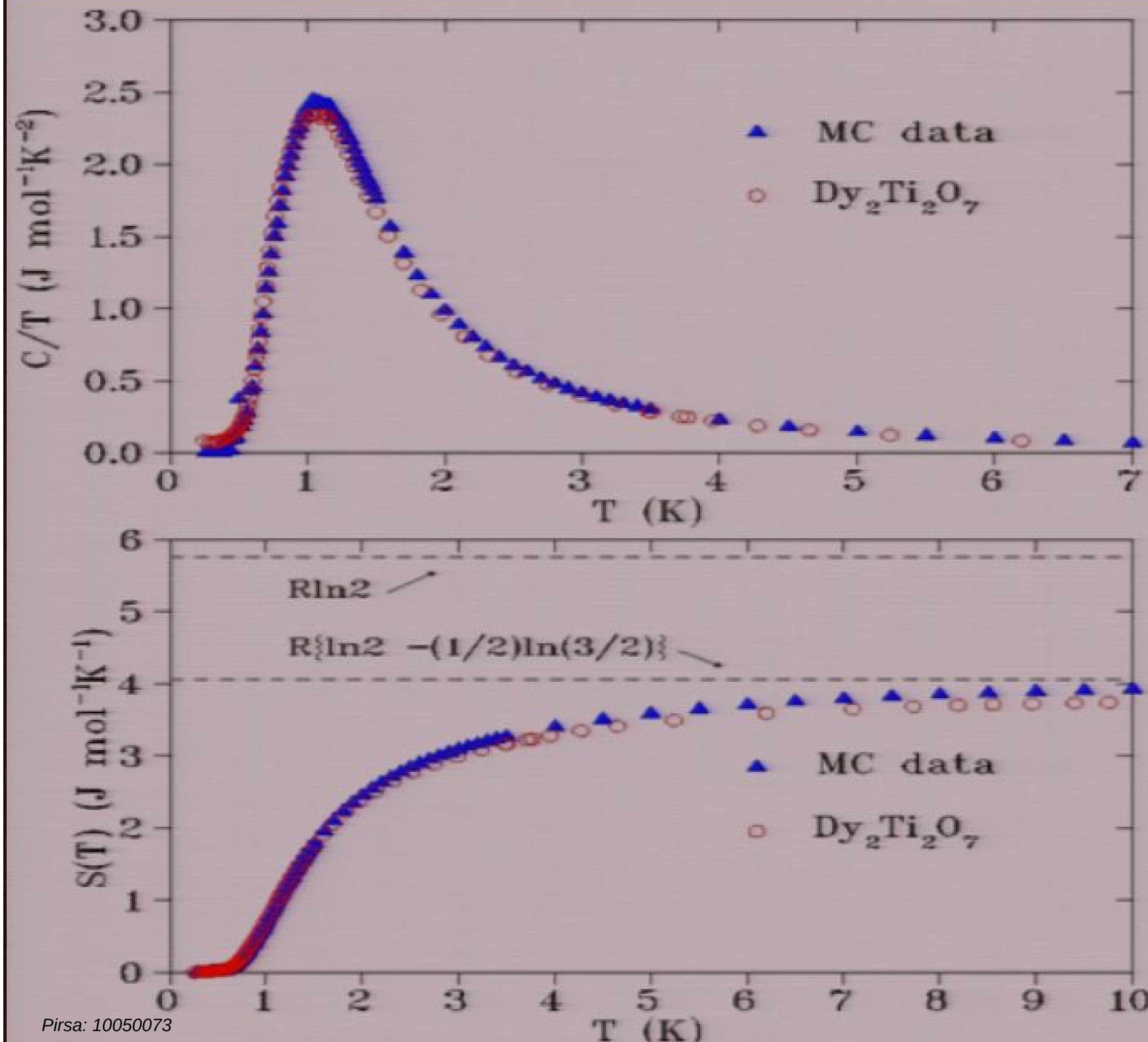
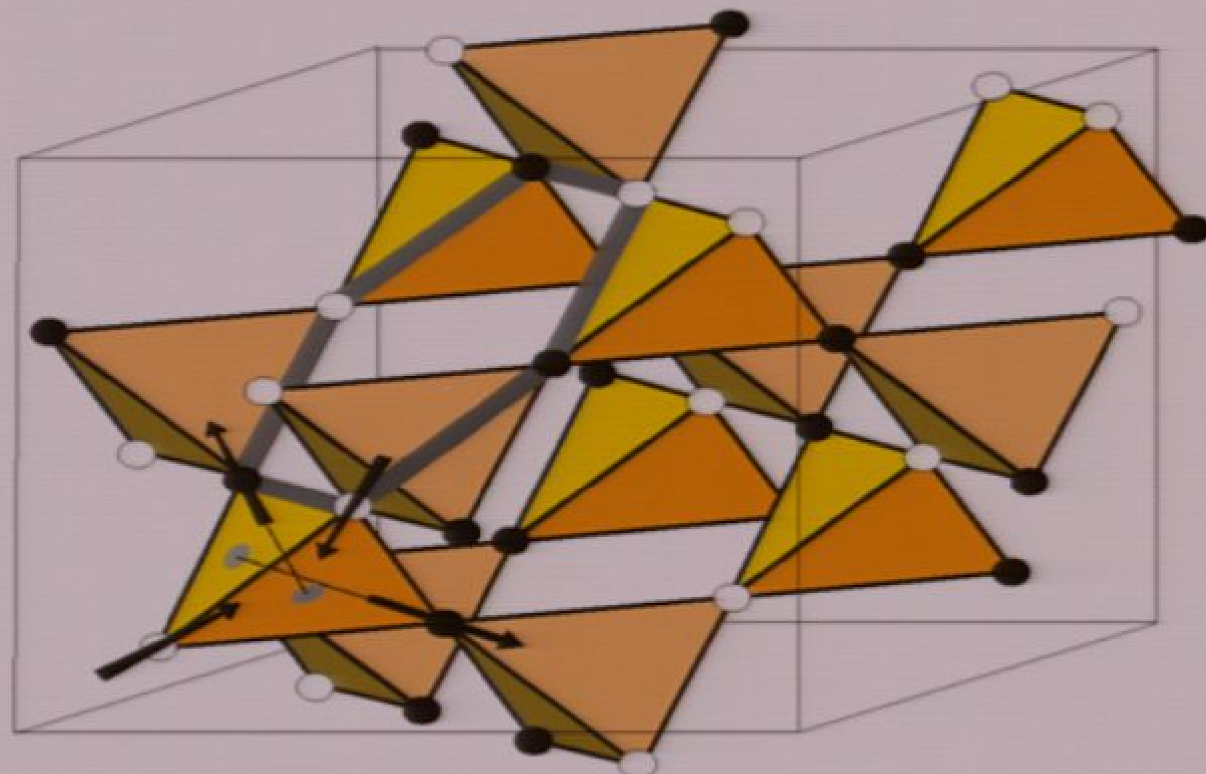


Nearest neighbor exchange:
$J_1 \sim -3.42\,\mathrm{K}$

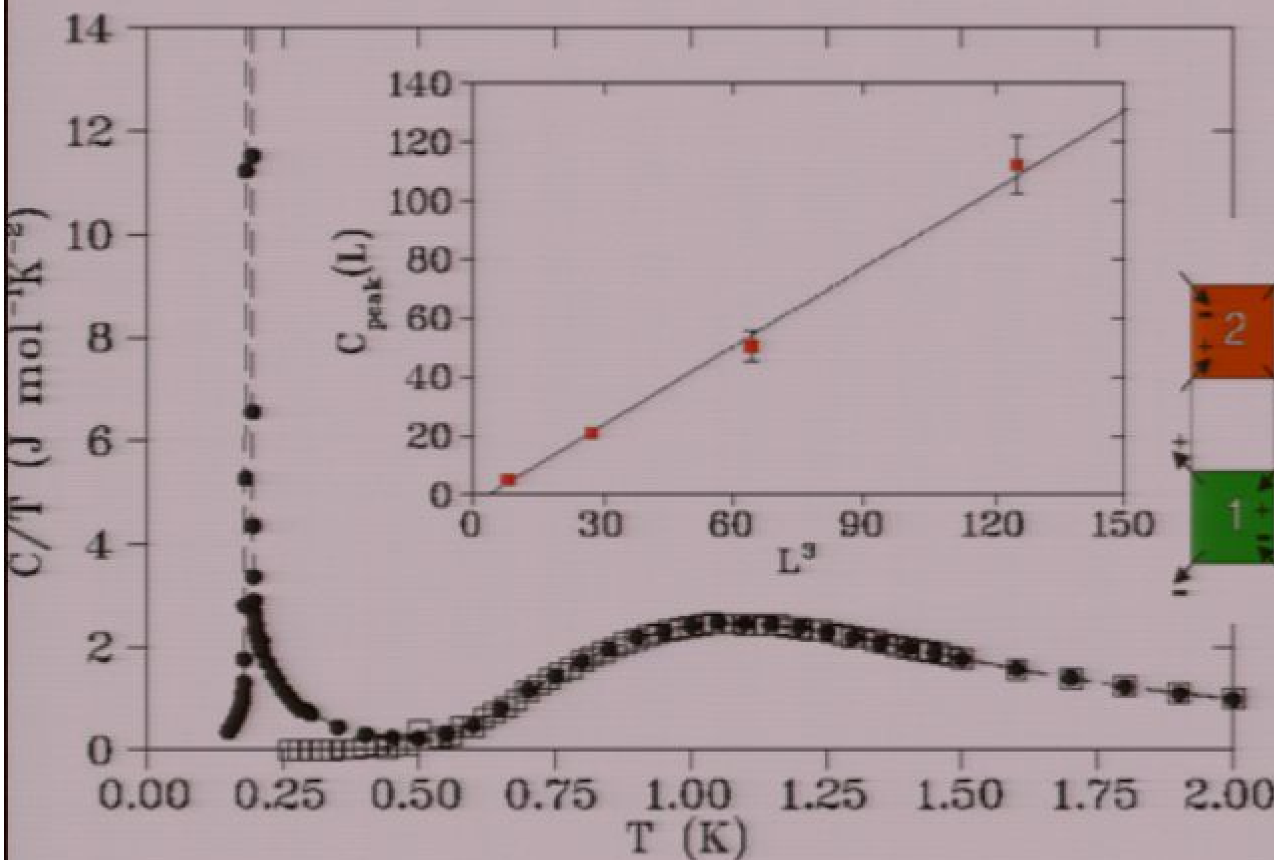
den Hertog and Gingras, *Phys. Rev. Lett.* **84**, 3430 (2000)

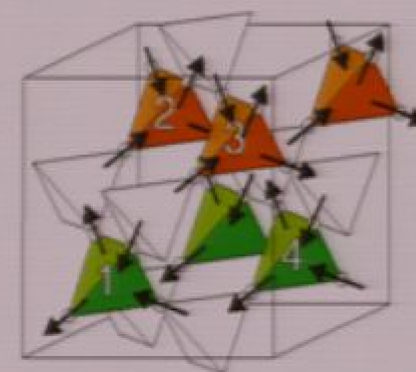
Energy Barriers and Loop Moves



Closed loops of spins can bypass the large energy barriers involved with flipping single spins, hence explore the quasi-degenerate spin ice manifold in "loop" Monte Carlo simulations.

- R. G. Melko, B. C. den Hertog, and M. J. P. Gingras, *Phys. Rev. Lett.* **87**, 067203 (2001).
- R. G. Melko and M.J.P. Gingras, J. Phys: Condens. Matt. **16**, R1277 (2004).
- S.T. Bramwell and M.J.P. Gingras, *Science* **294**, 1495 (2001).



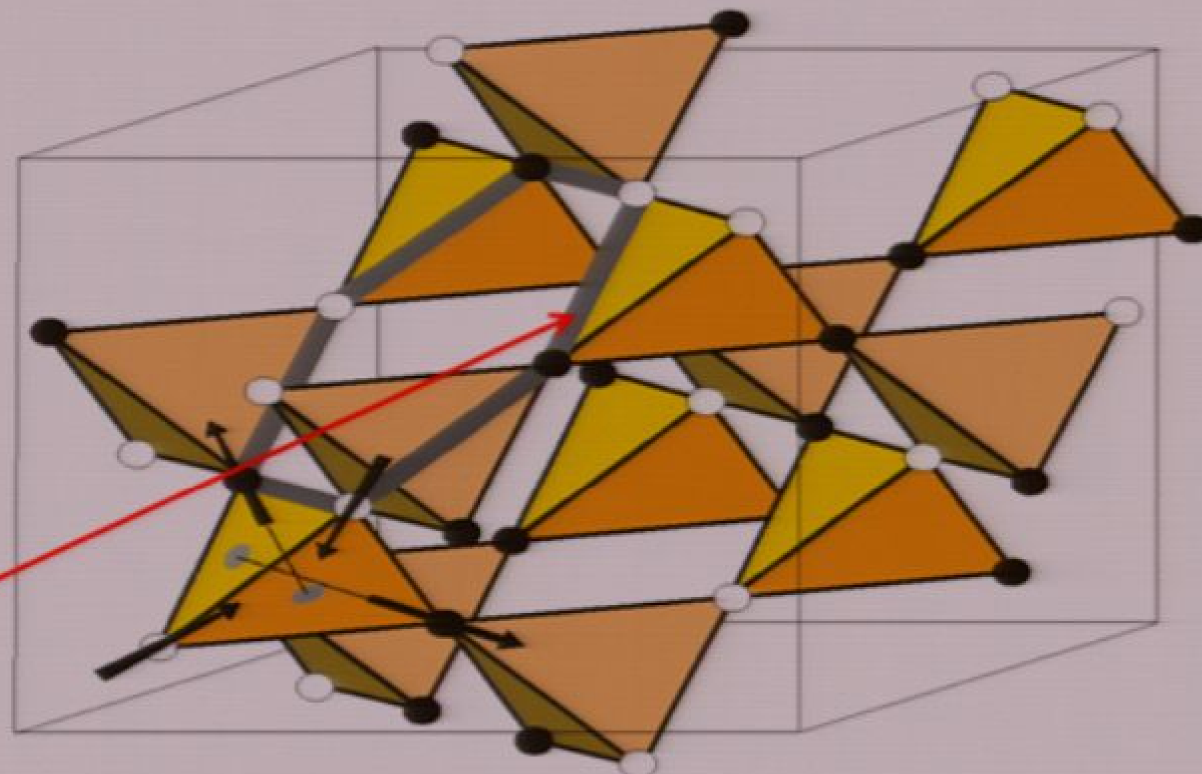


By removing the energy barriers associated with single spin flips, we have allowed the system to select a unique long range ordered ground state.

$$\mathbf{q} = (0, 0, 2\pi / a)$$

Same ordering as in mean field theory /Gaussian approximation (Gingras and den Hertog, Can. J. Phys. **79**, 1339 (2001).

Energy Barriers and Loop Moves



Also referred to as "Dirac strings" in more recent discussions

Closed loops of spins can bypass the large energy barriers involved with flipping single spins, hence explore the quasi-degenerate spin ice manifold in "loop" Monte Carlo simulations.

- R. G. Melko, B. C. den Hertog, and M. J. P. Gingras, *Phys. Rev. Lett.* **87**, 067203 (2001).
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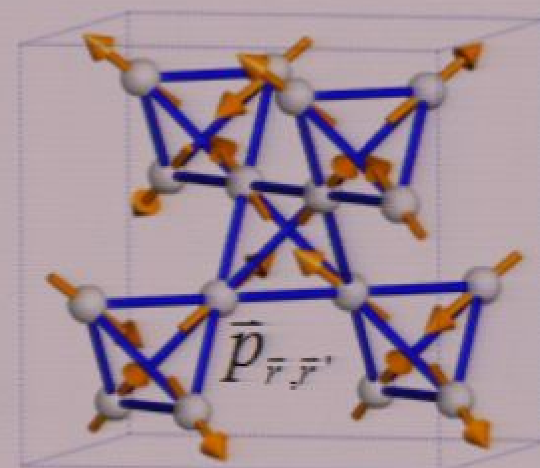
- S.T. Bramwell and M.J.P. Gingras, *Science* **294**, 1495 (2001).

Outline

1. **Introduction – a review of spin ice physics**
   - *Frustrated ferromagnet & ice rules*
   - *extensive low-temperature entropy*
   - *role of dipolar interactions*
2. **Spin ice – recent developments**
   - *Coulomb phase and divergence free field*
   - *Spin-spin correlations*
   - *Excitations in the Coulomb phase and monopoles*
   - *Magnetic-field induced dissociation of ice rules*
3. **Spin liquid physics of $Tb_2Ti_2O_7$**
   - *Corrections to Ising model*
   - *"Quantum spin ice"*
4. **Conclusion**

3. Coulomb phase physics

- The spin ice rule can be mapped in the long length scale limit to a non-divergent (polarization) field that lives on the "parent" diamond lattice



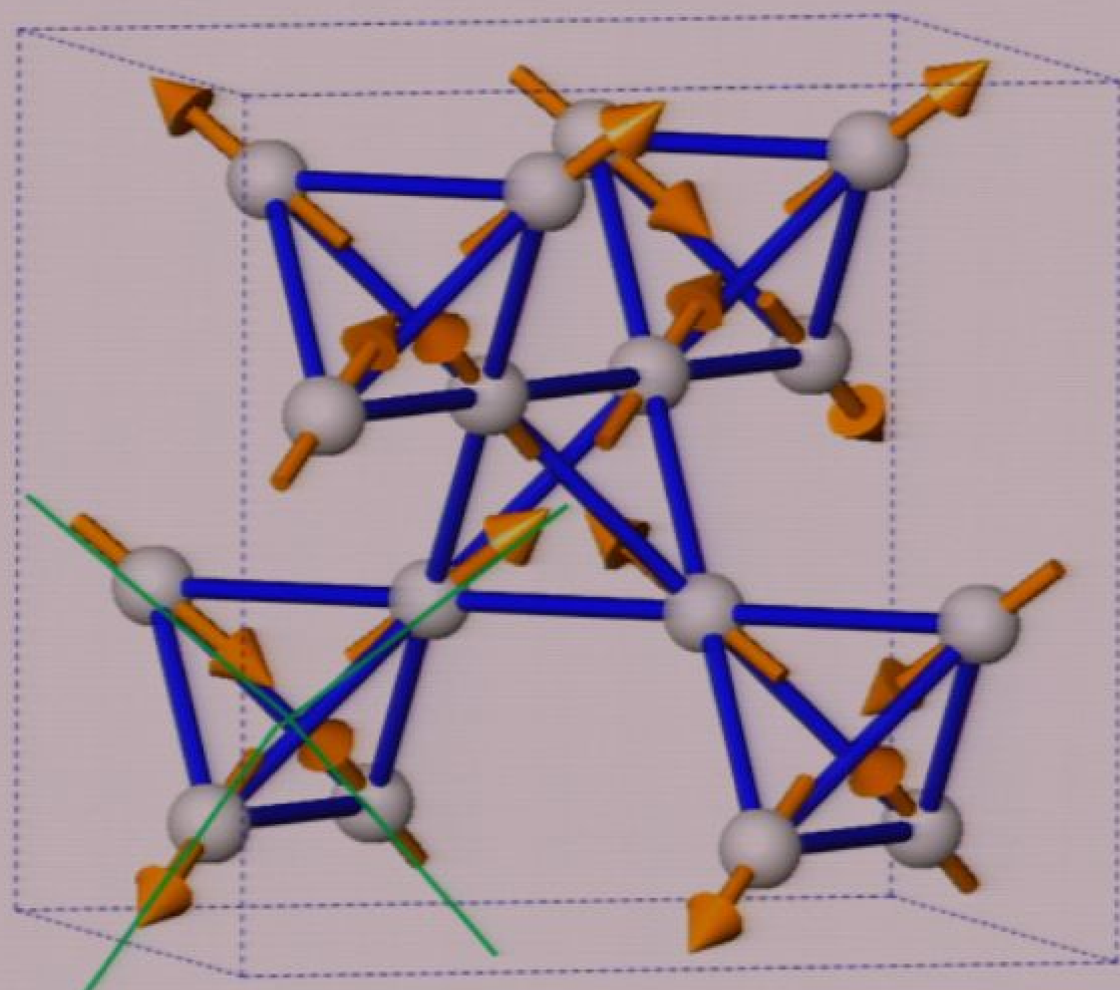
$$\nabla \bullet \vec{P} = 0$$

- The excitations (spin flip) that break the ice rule create effective "*charges*".
- The system obeys a *"magnetic Gauss' Law"* which relates the density ρ of defects in the P field

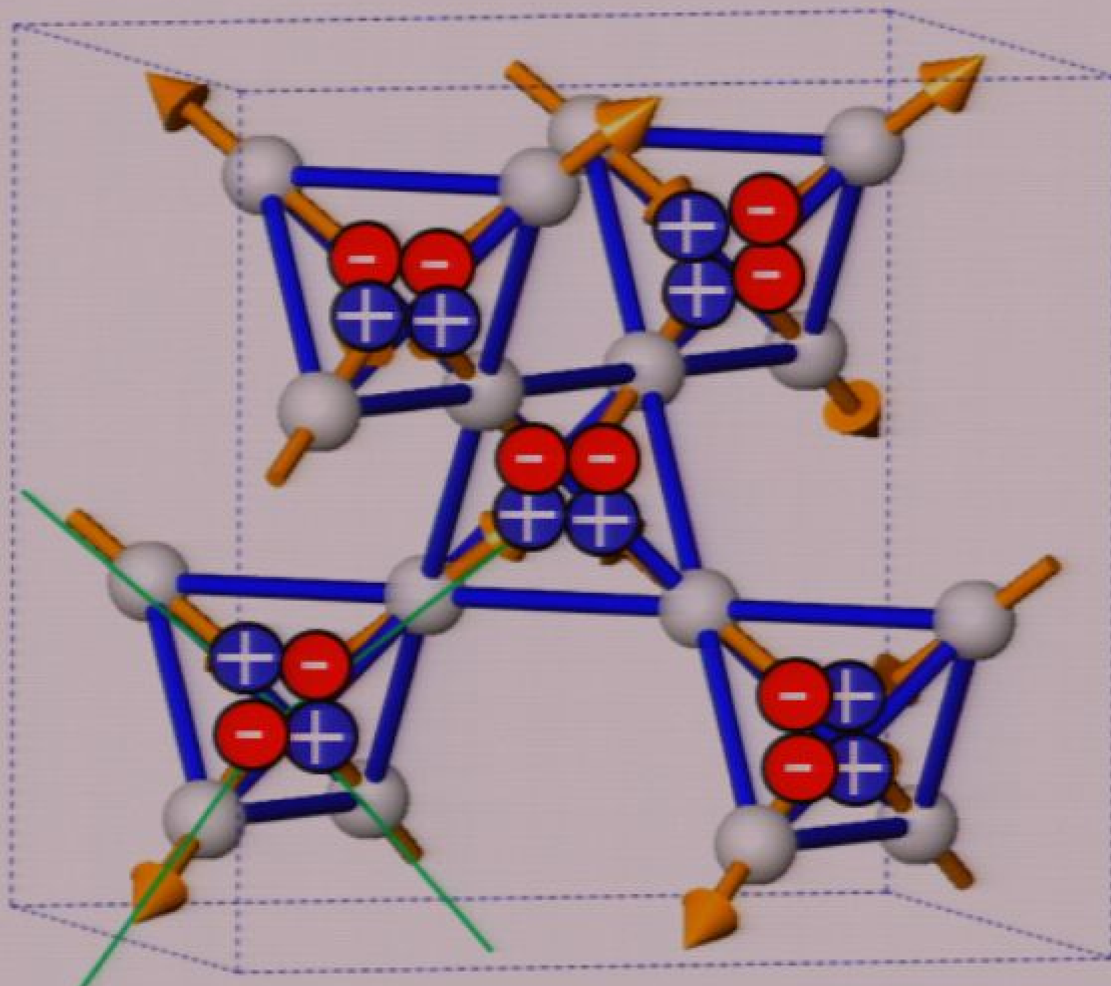
$$\nabla \bullet \vec{P} \propto \rho$$

Castelnovo *et al.*, Nature **451**, 41 (2008).

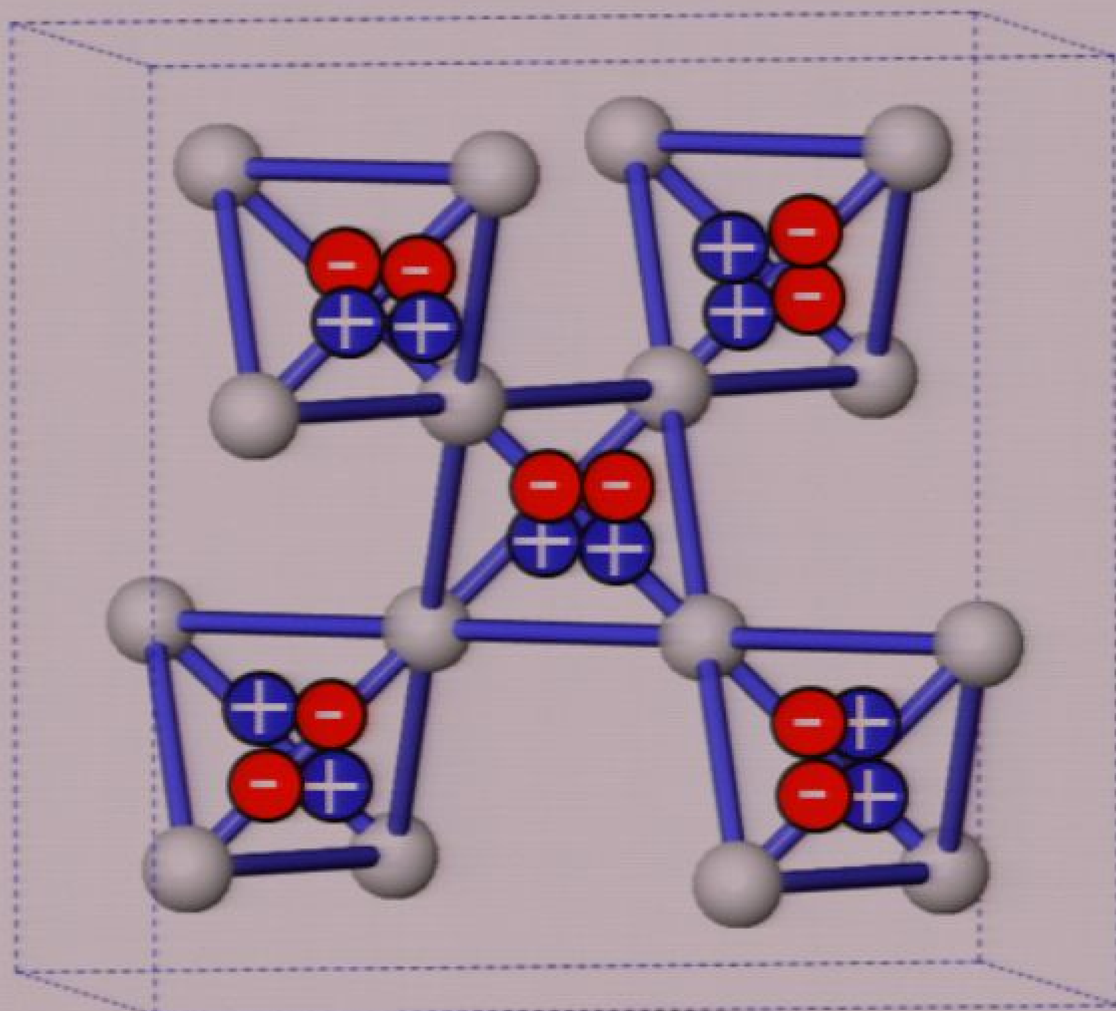
“Two-in/two-out” ice rules



“Two-in/two-out” ice rules



"Two-in/two-out" ice rules



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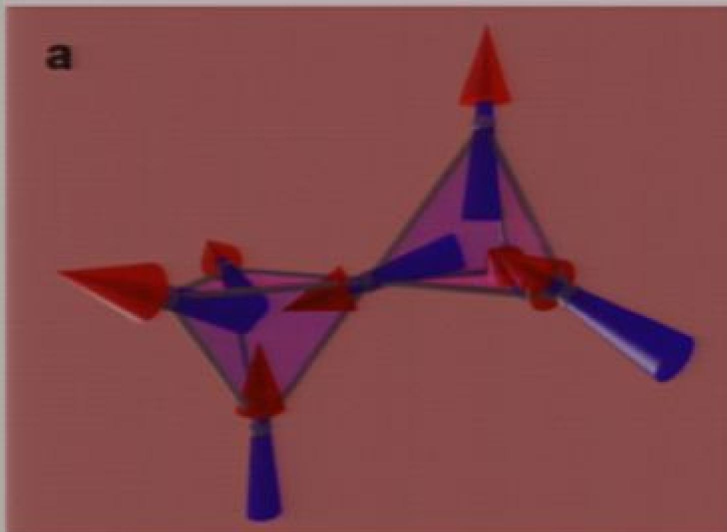

Castelnovo *et al.*, Nature **451**, 41 (2008).

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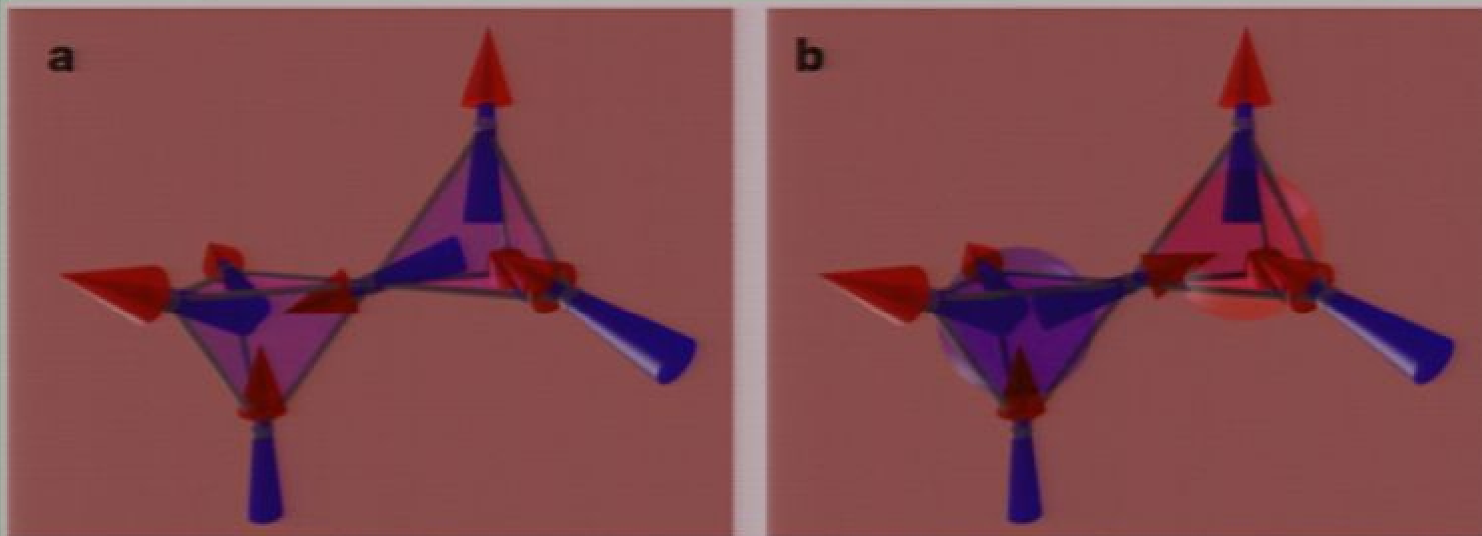

Castelnovo *et al.*, Nature **451**, 41 (2008).

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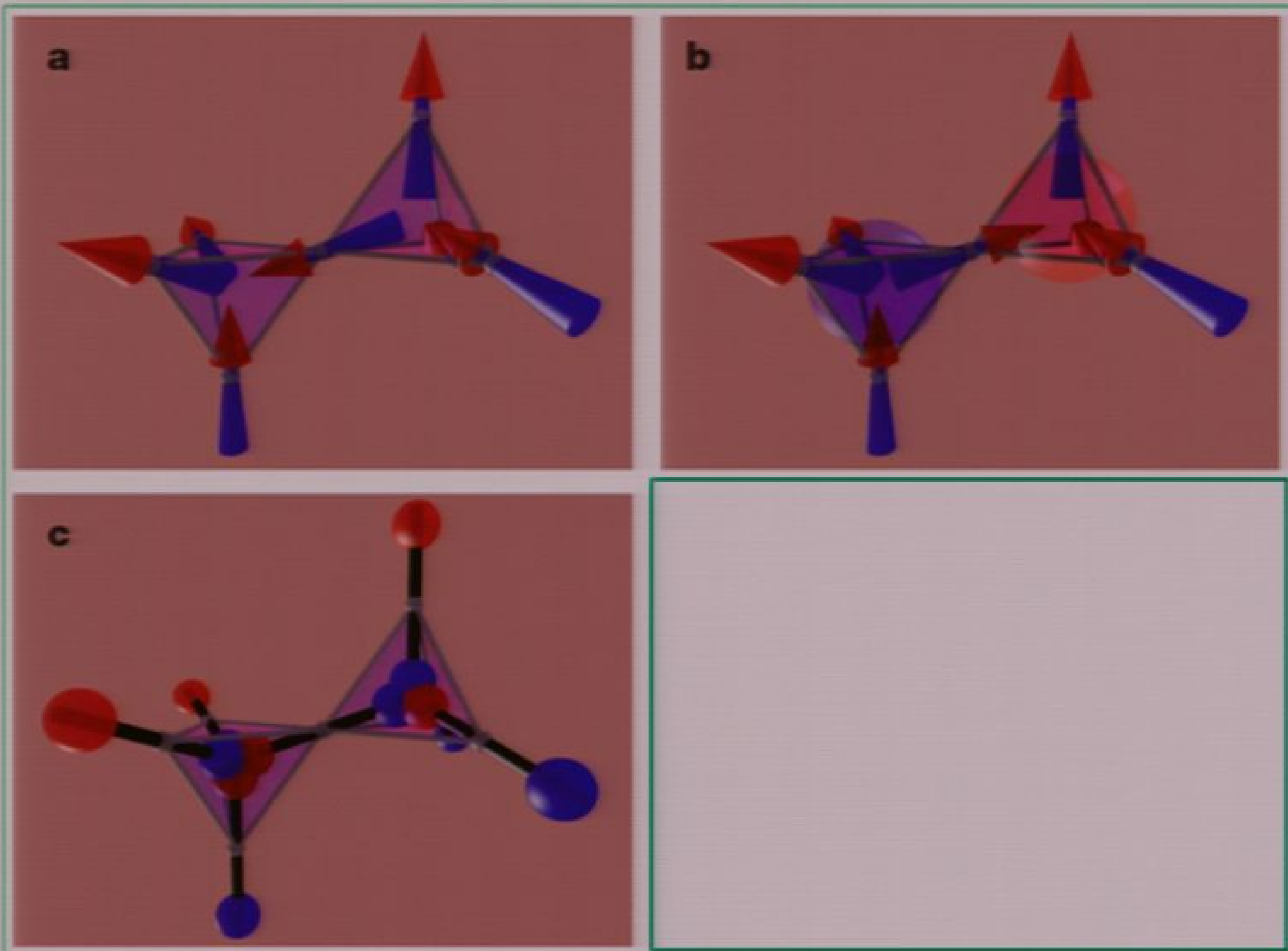

Castelnovo *et al.*, Nature **451**, 41 (2008).

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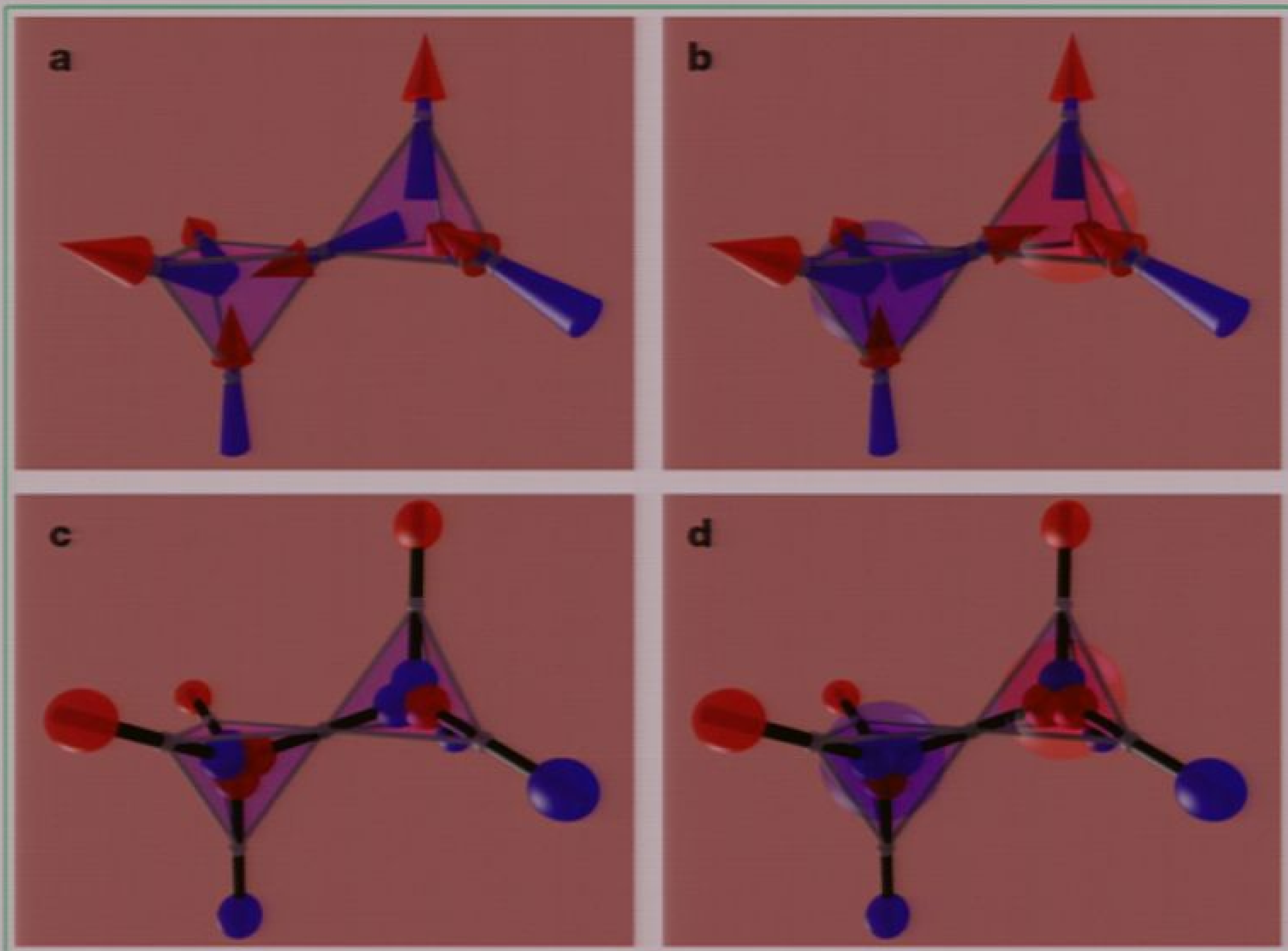

Castelnovo *et al.*, Nature **451**, 41 (2008).

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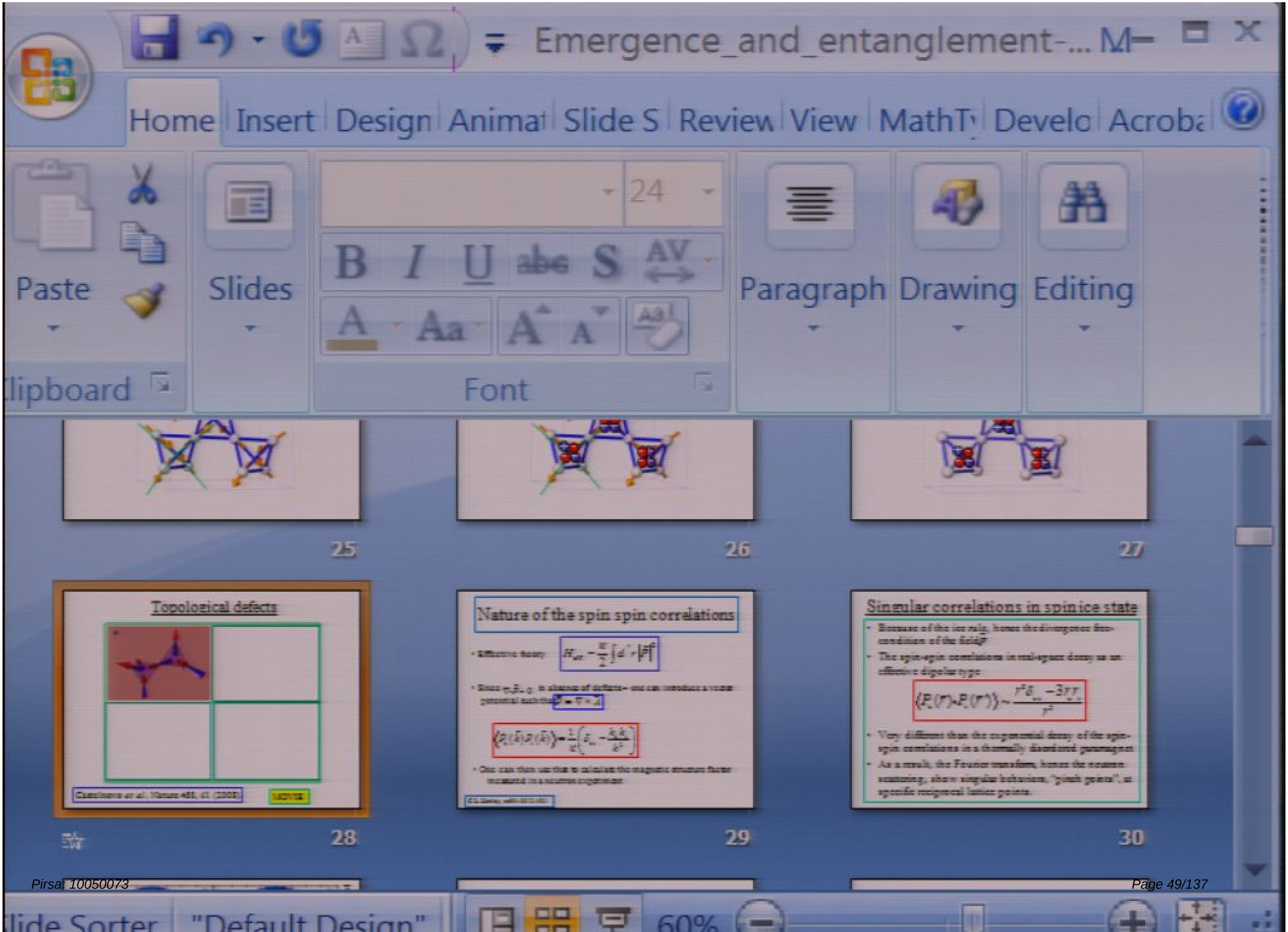
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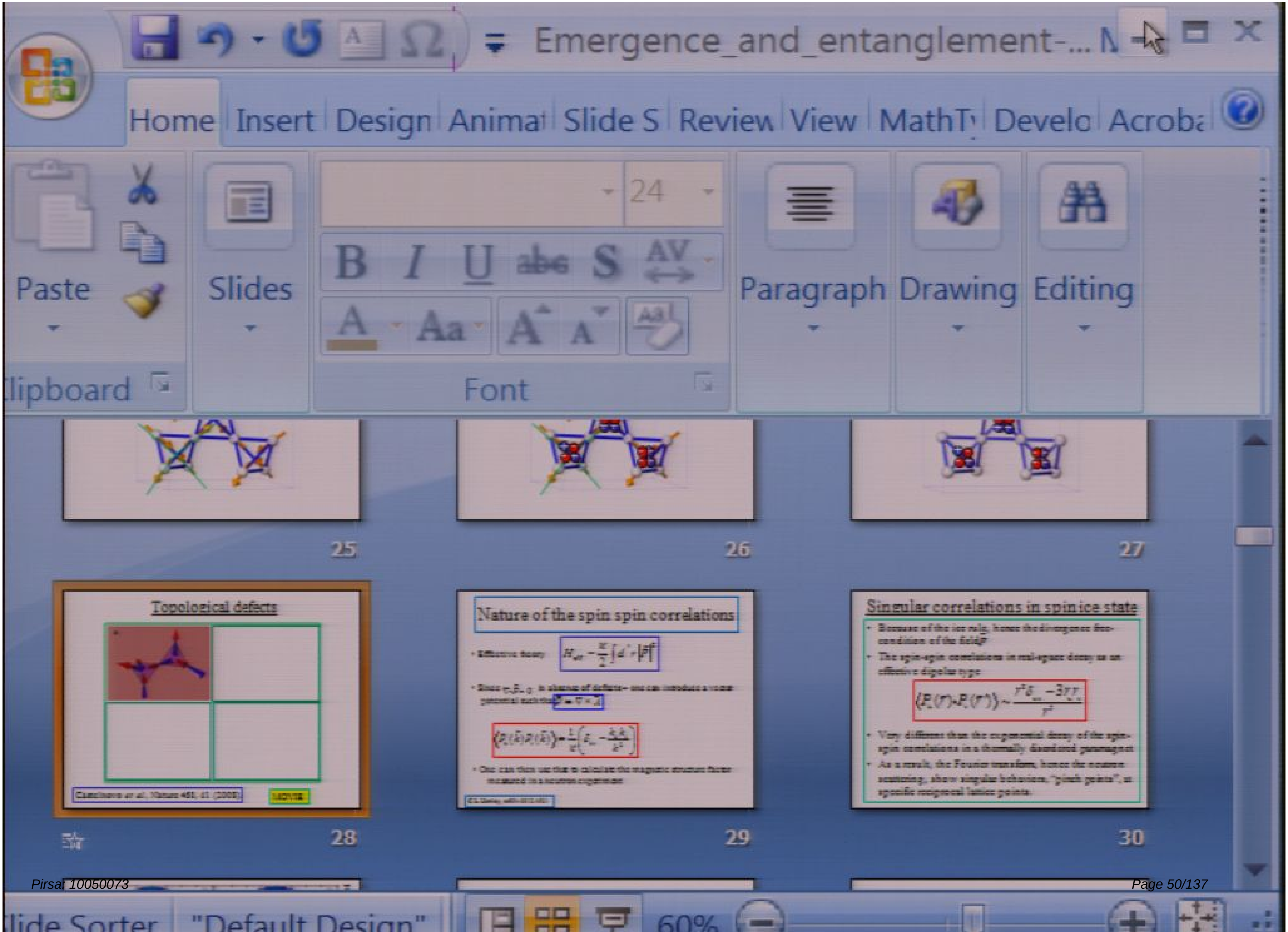

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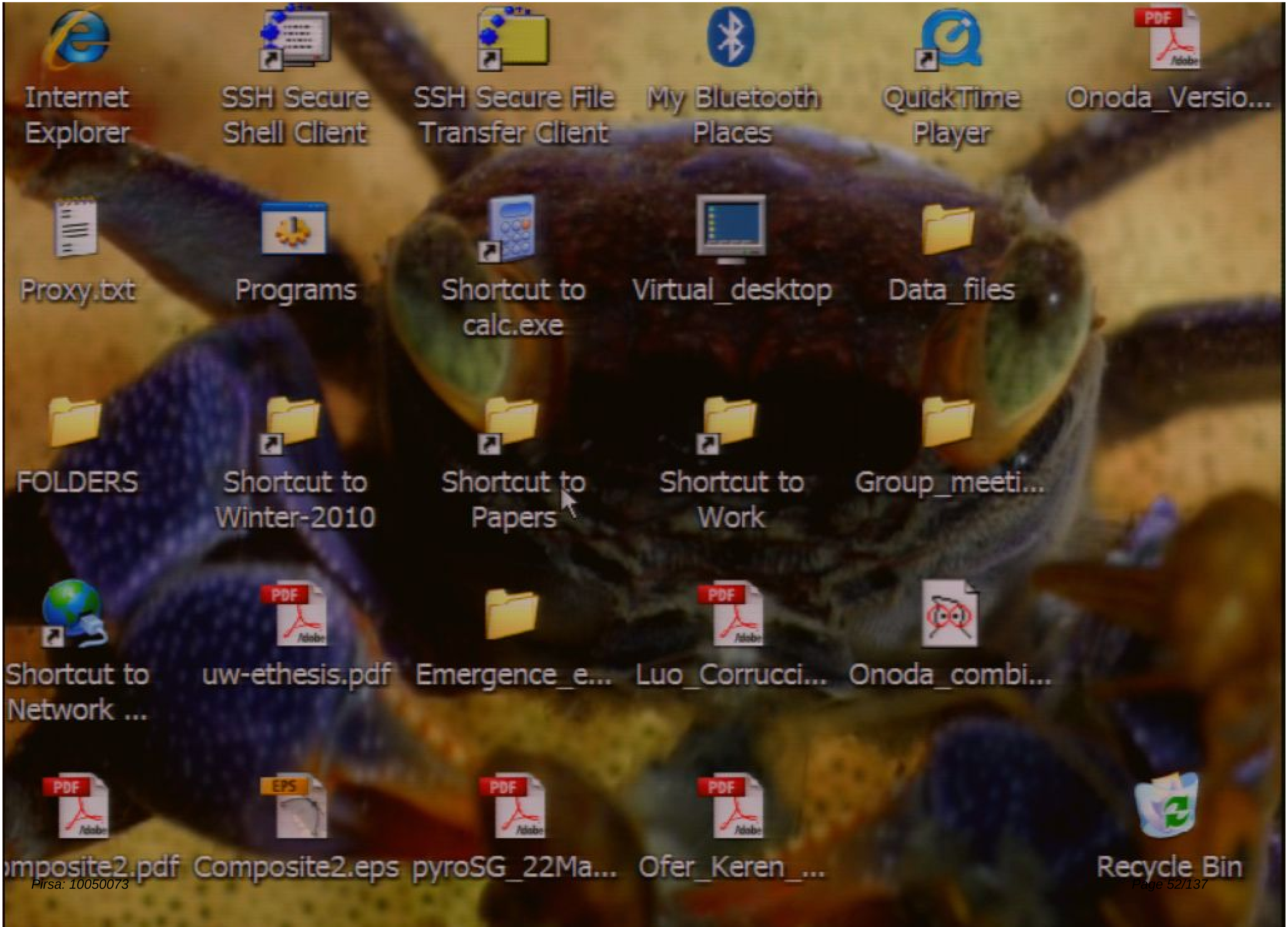
rare-eath ions with fewer f electrons, the $4f$ wavefunction is spatially expanded [10] and can then be largely overlapped with the O $2p$ orbitals at the O1 site (Fig. 1 (a)) in the pyrochlore lattice. Besides, for Pr^{3+} ions, the magnetic dipolar interaction, which is proportional to the square of the moment size, is reduced by an order of magnitude to 0.1 K between the nearest-neighbor sites, in comparison to that for Dy^{3+} ions. Then, the superexchange interaction due to virtual f-p electron transfers, which provides a source of the quantum nature, is expected to play crucial roles in $Pr_2TM_2O_7$ (TM: transition-metal element).

Recent experiments on $Pr_2Sn_2O_7$ [11], $Pr_2Zr_2O_7$ [12], and $Pr_2Ir_2O_7$ [13] have shown that the Pr^{3+} ion provides the $\langle 111 \rangle$ Ising moment described by a non-Kramers magnetic doublet. As in the spin ice, any magnetic dipole

other hand, the Curie-Weiss temperature T_{CW} is antiferromagnetic for the zirconate [12] and iridate [13], unlike the spin ice. The stannate shows a significant level of low-energy short-range spin dynamics [15], which is absent in the classical spin ice. Furthermore, the iridate shows the Hall effect at zero magnetic field without magnetic dipole order [14], suggesting an onset of a chiral spin-liquid phase [3] at a temperature $\sim J$.

In this Letter, we propose a novel scenario of the quantum melting of the spin ice, which can explain experimentally observed magnetic properties in $Pr_2TM_2O_7$. We uncover that a realistic minimal model derived for Pr $4f$ magnetic moments on the pyrochlore lattice shows a cooperative ferroquadrupole order. This is accompanied by crystal symmetry lowering from cubic to tetragonal and can be categorized into a spin smectic order [16]. We also reveal a frustration in the chirality ordering.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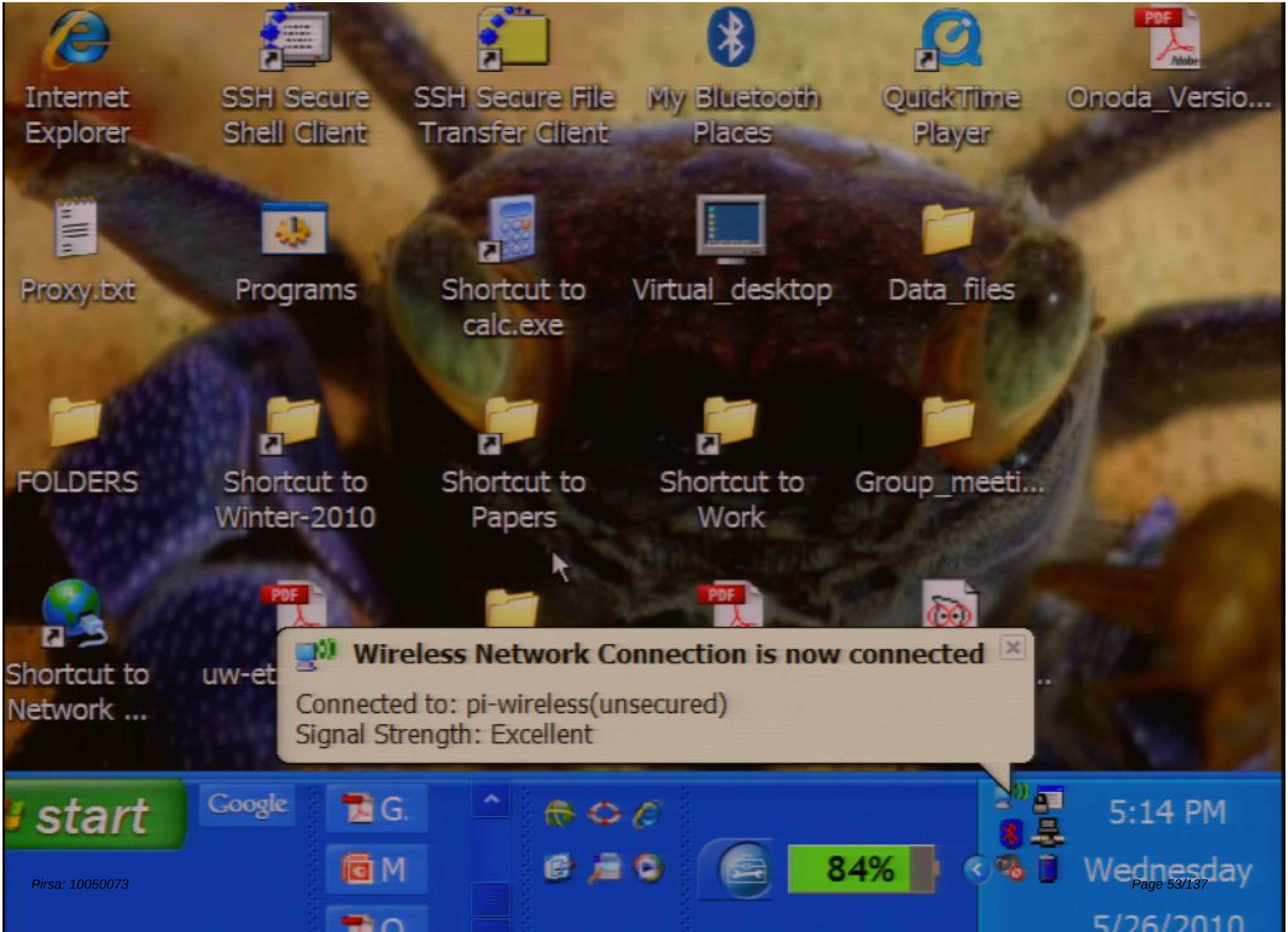
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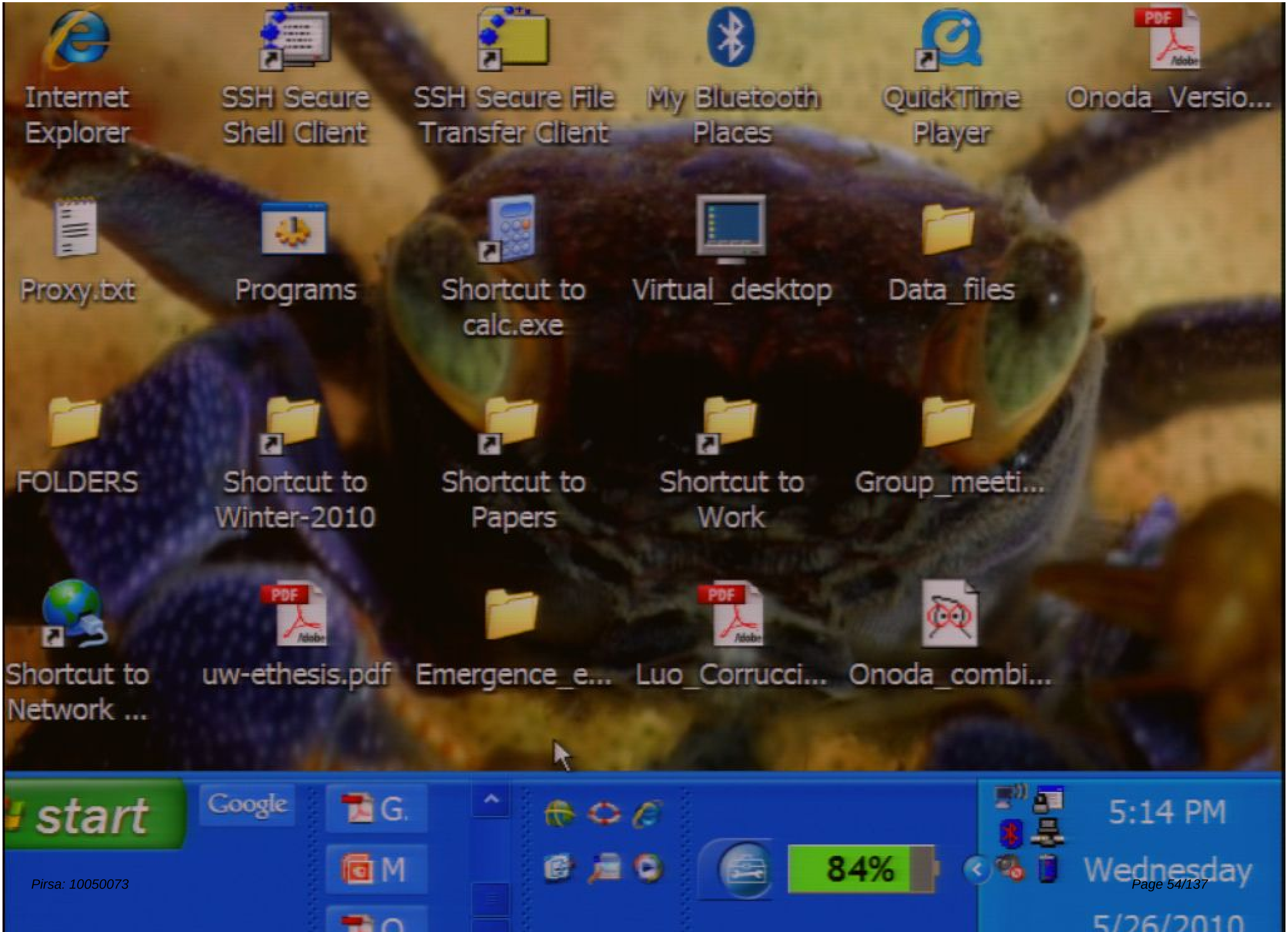
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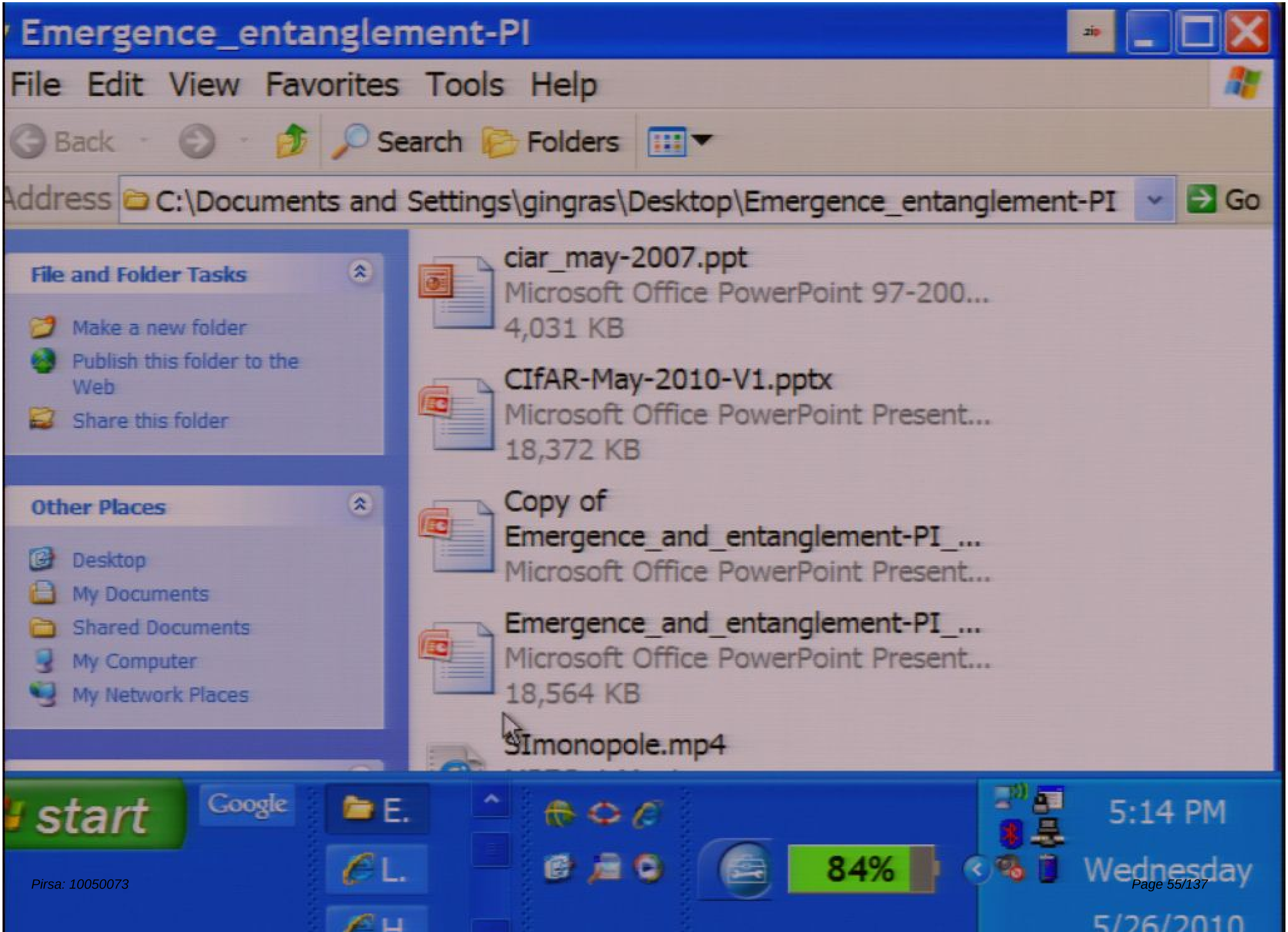
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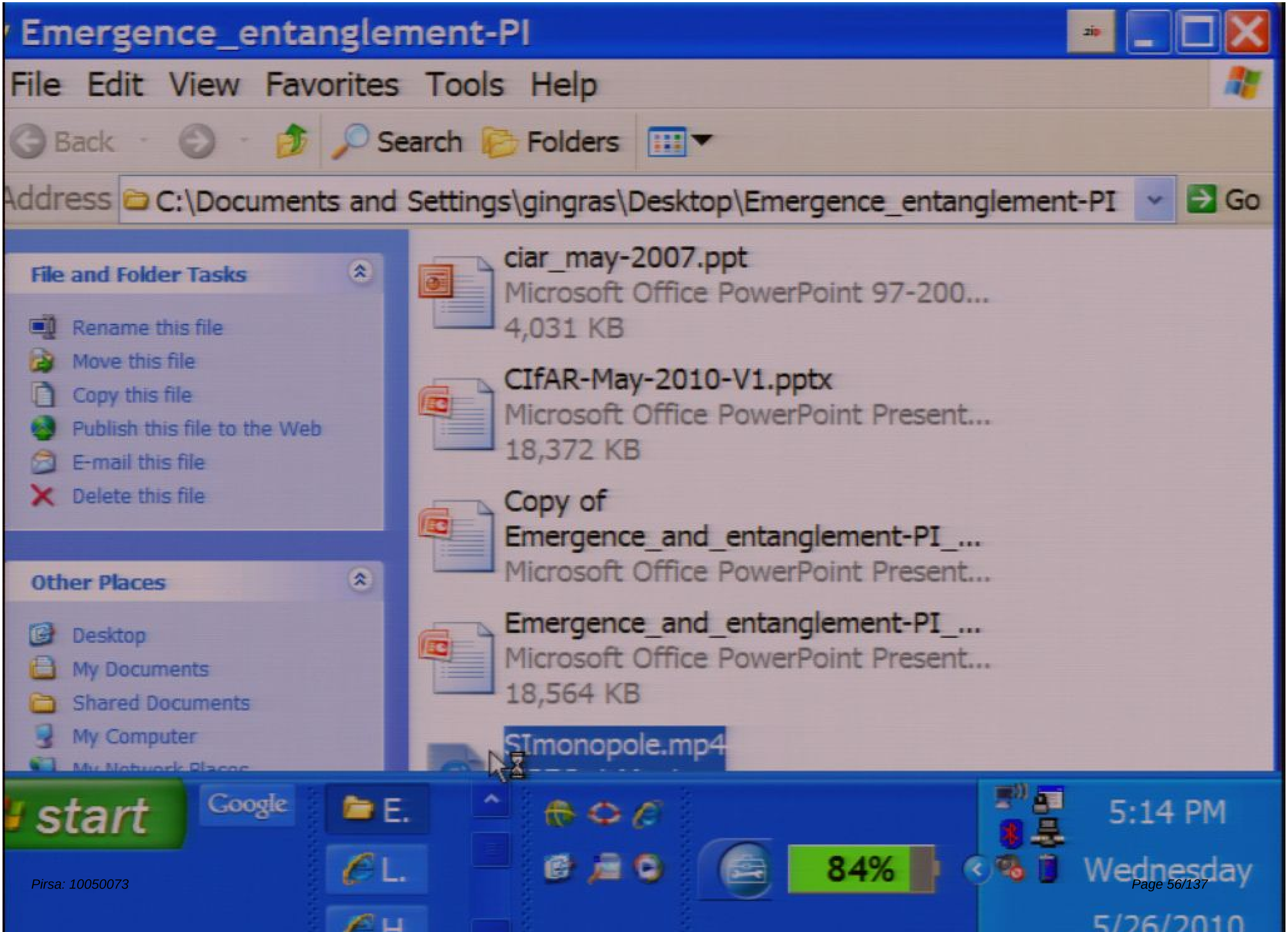
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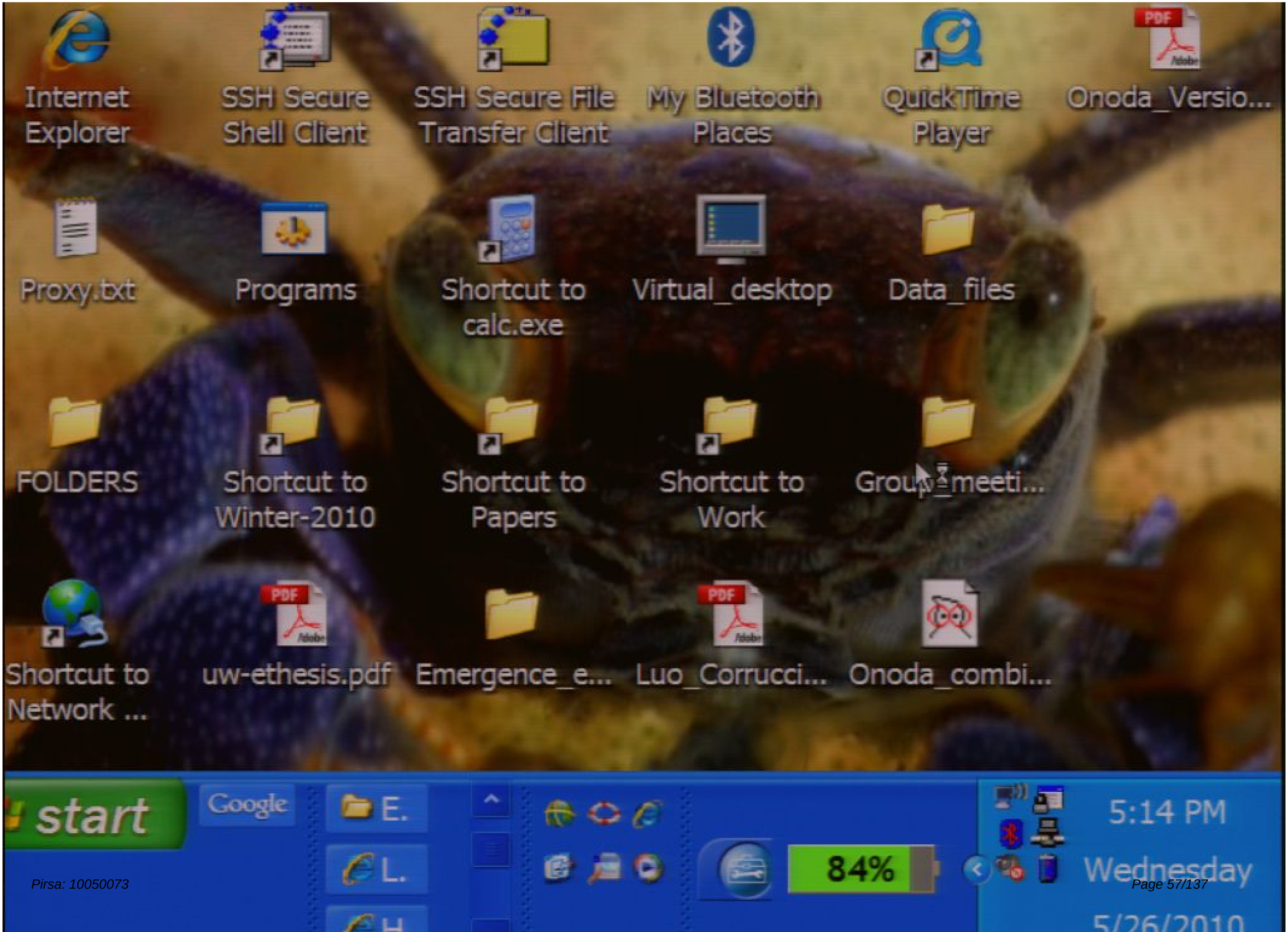
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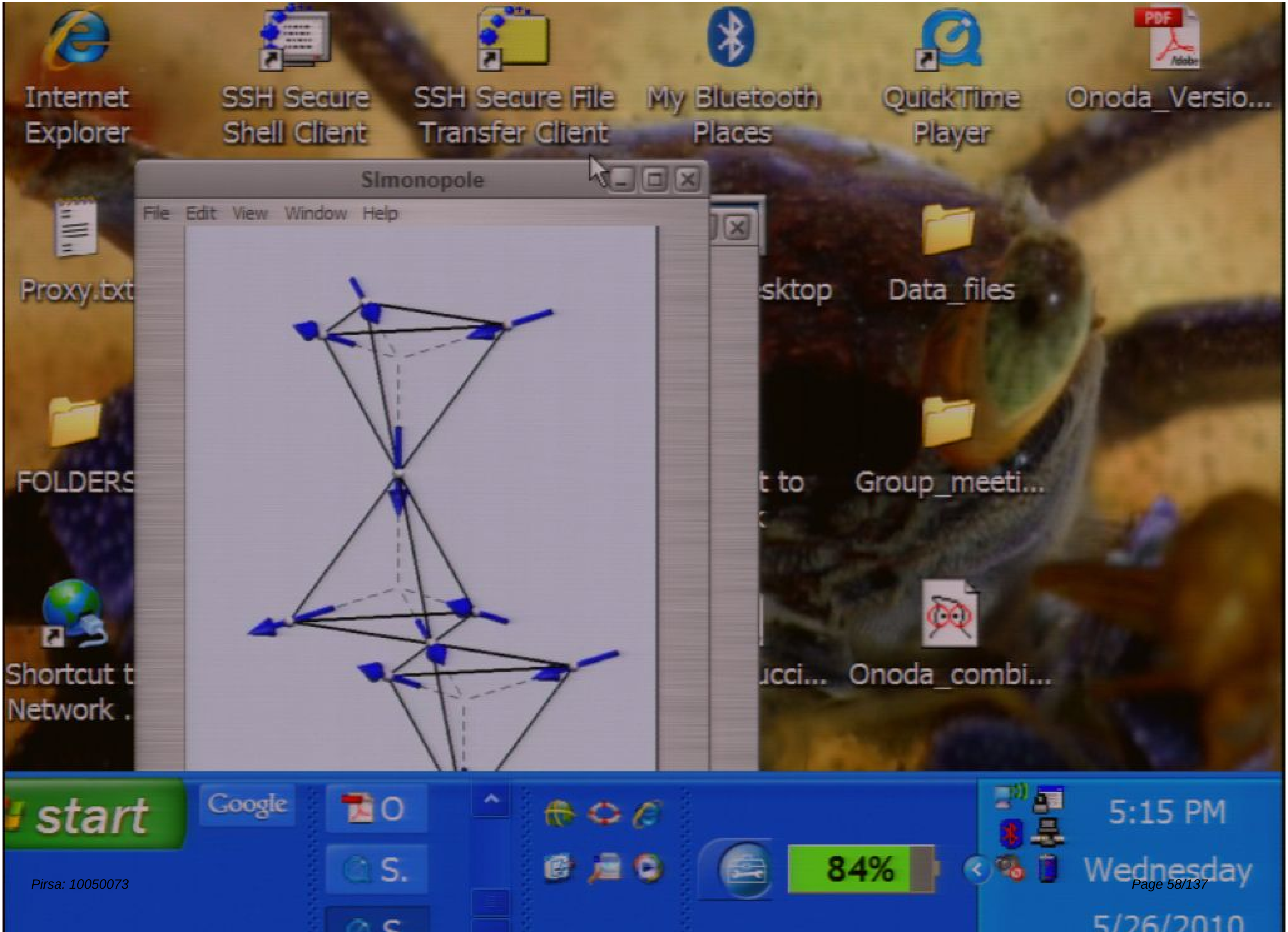

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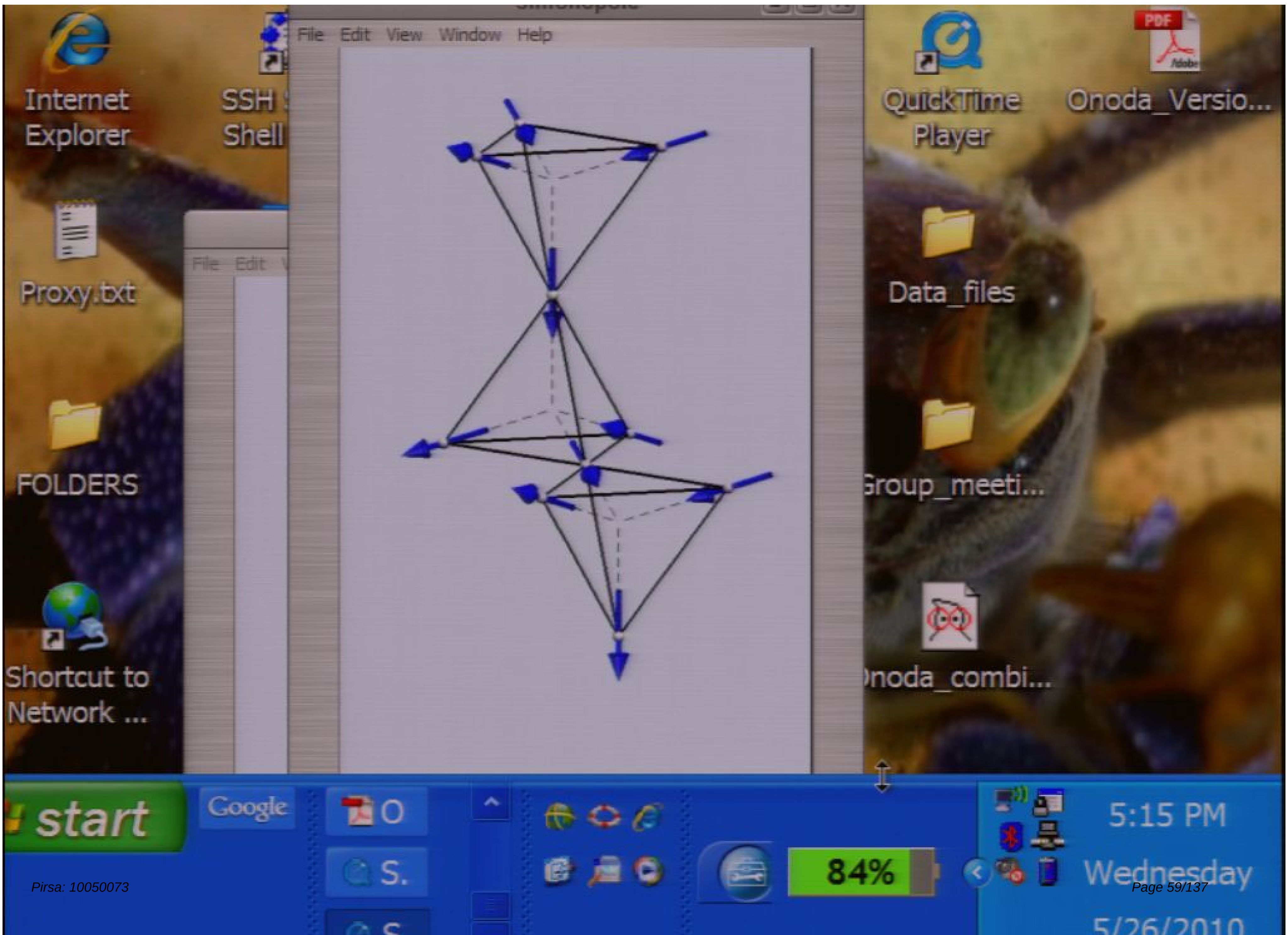

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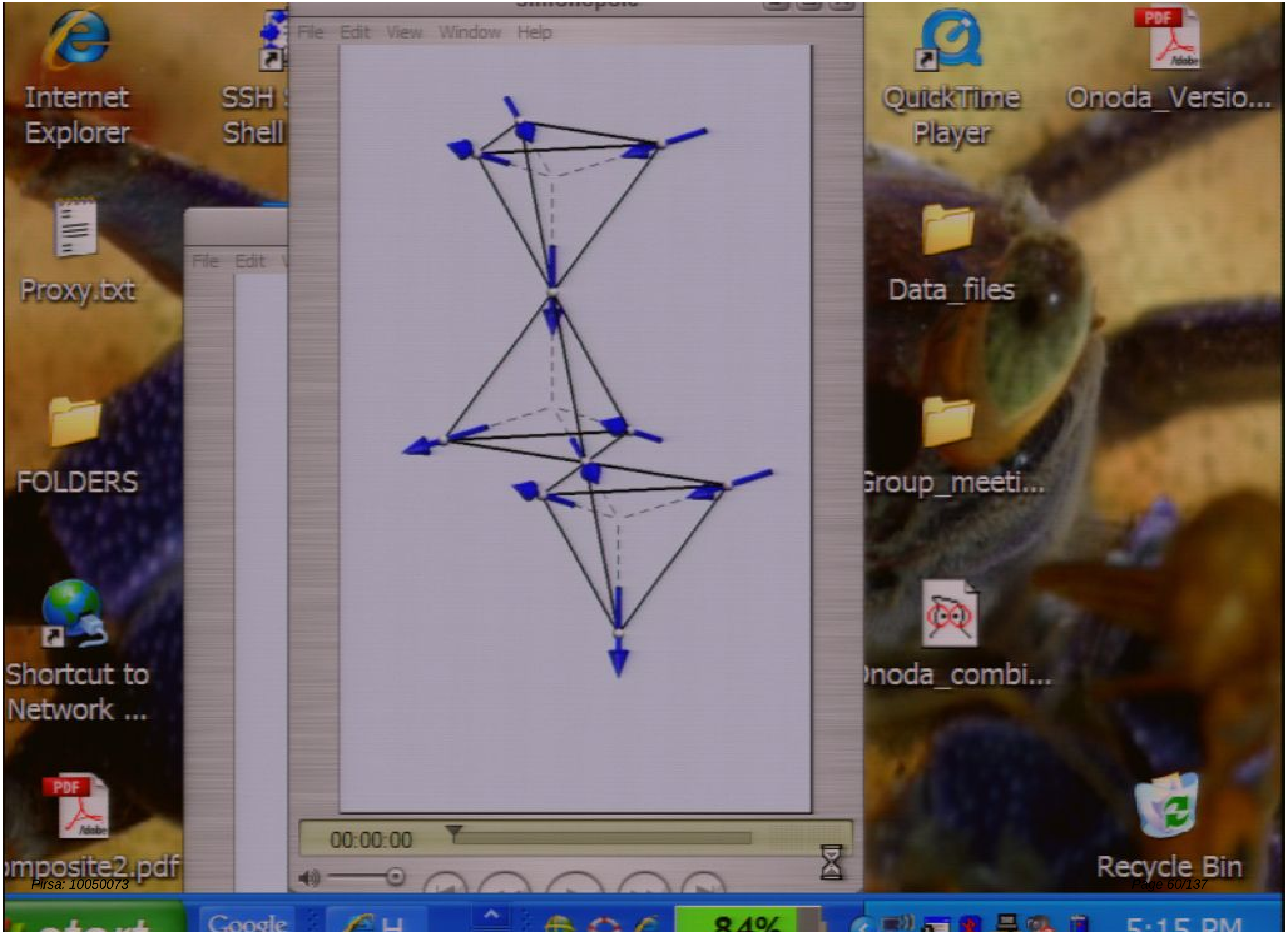
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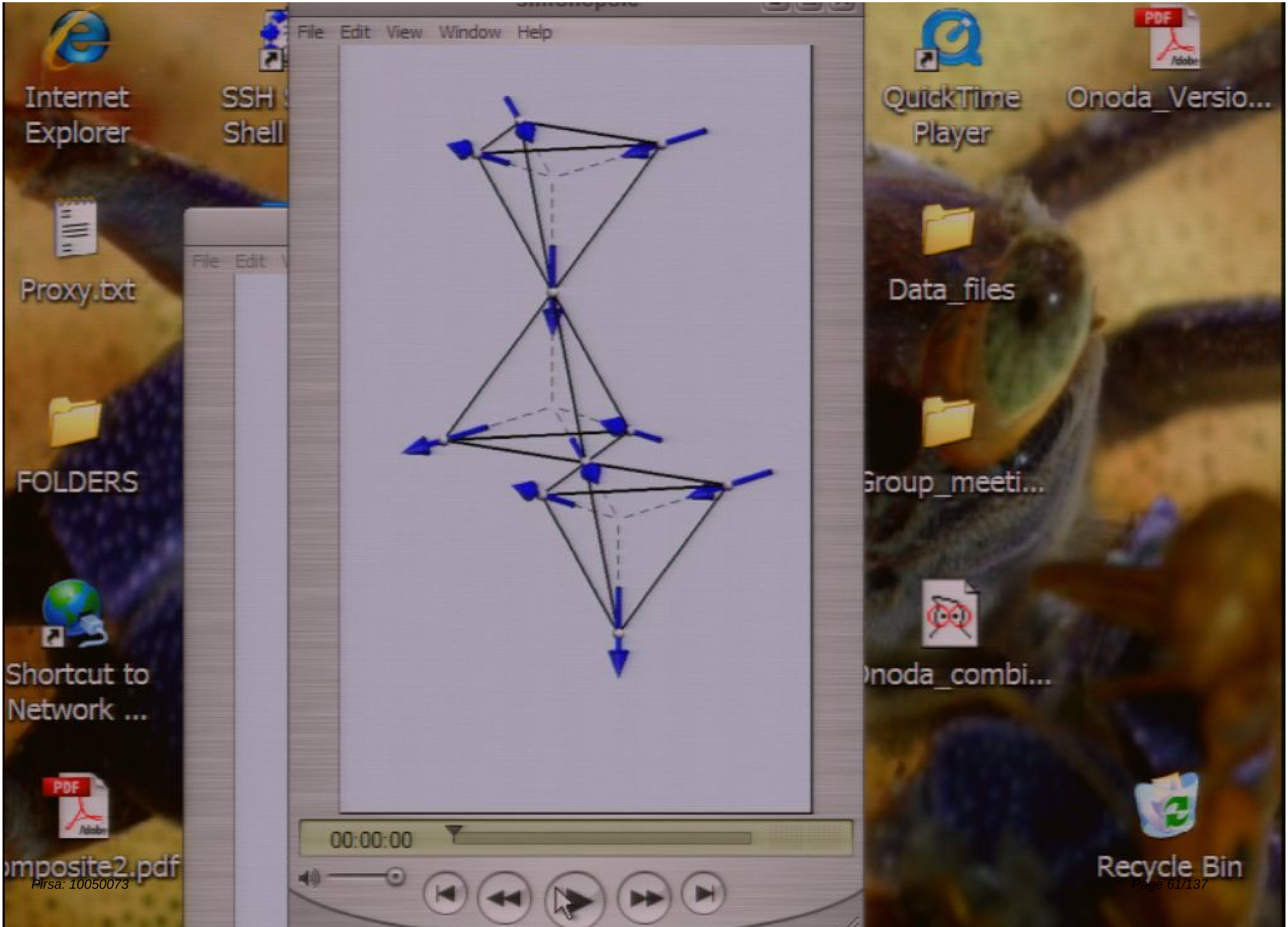
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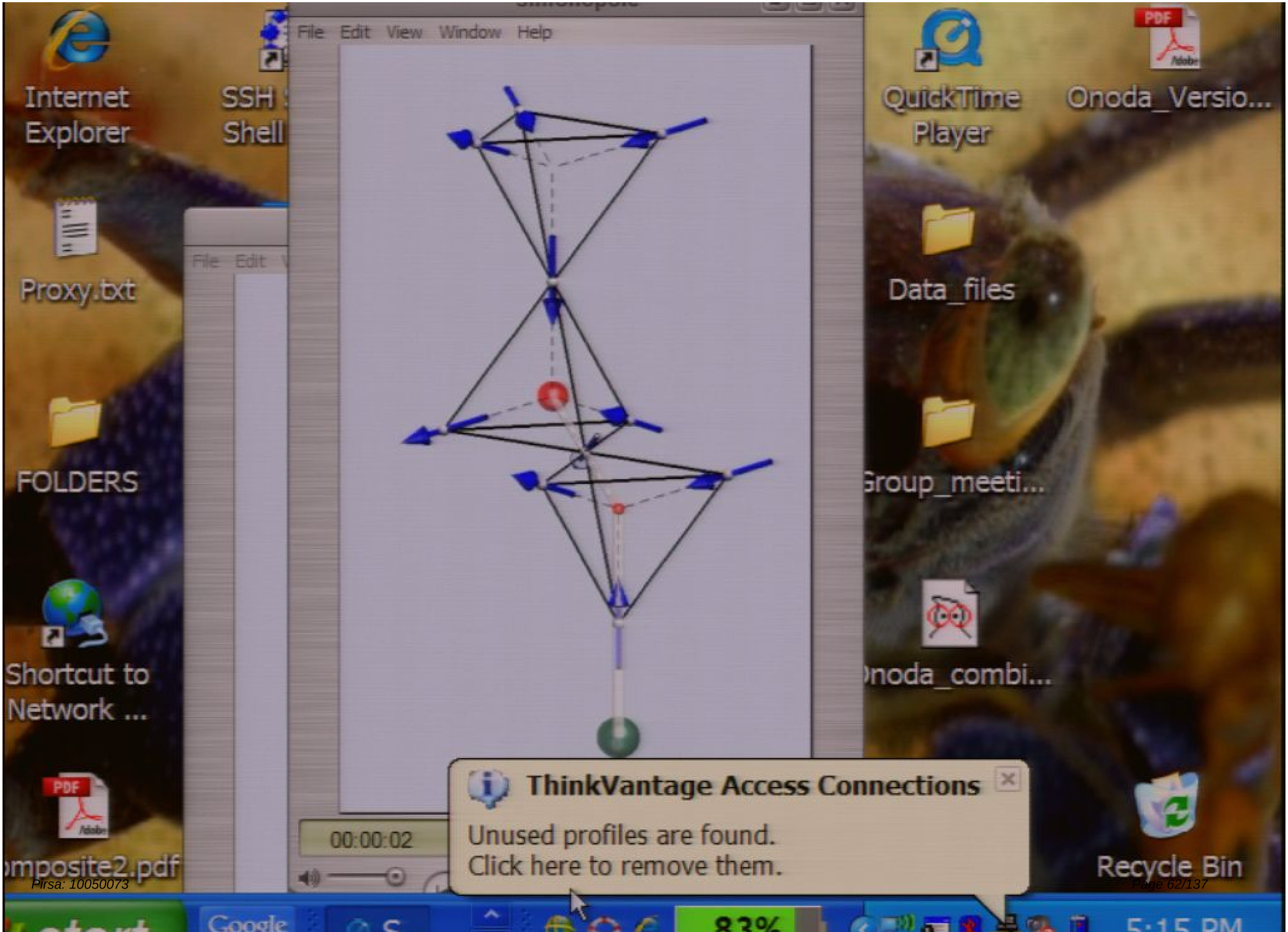
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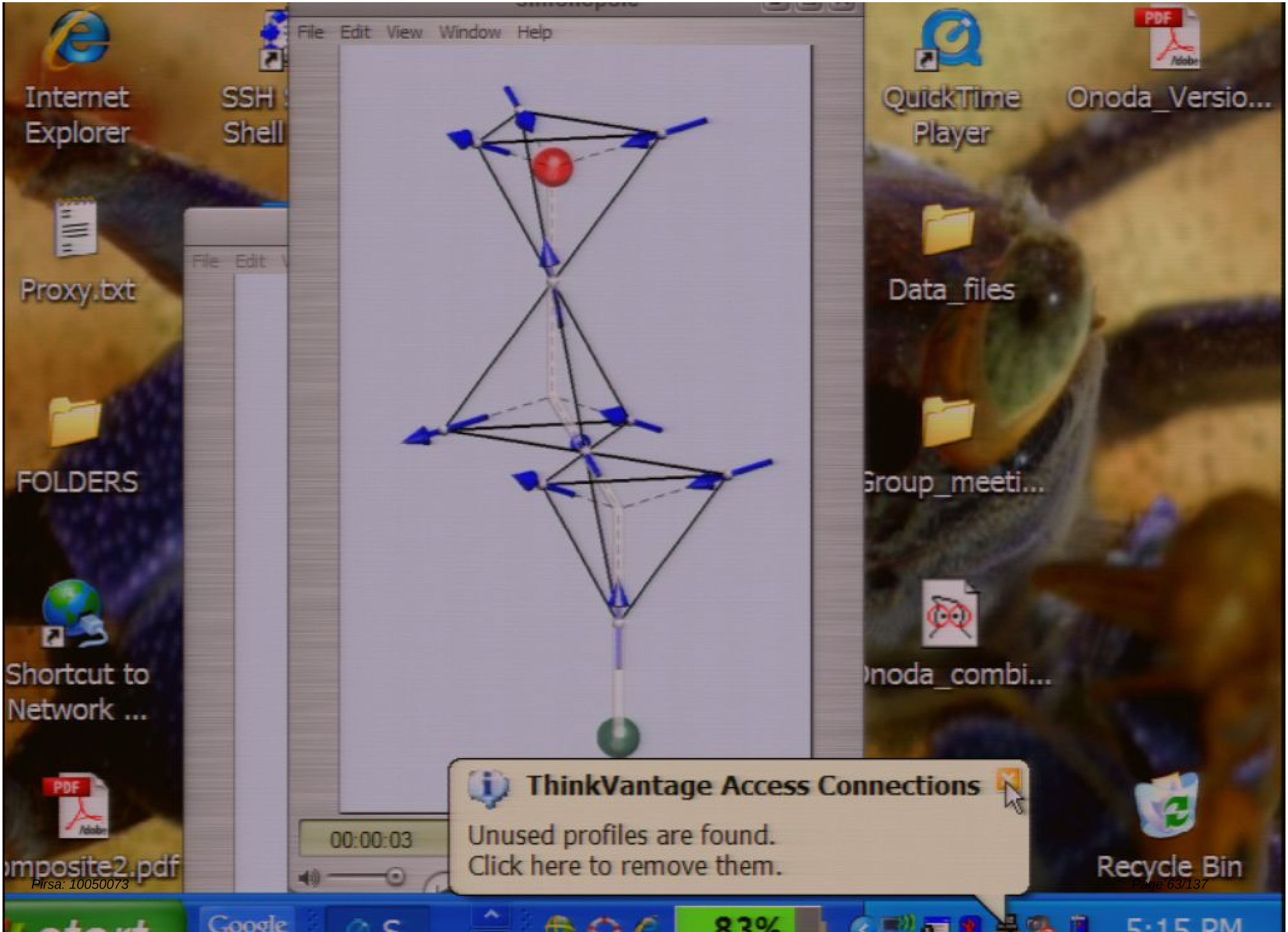
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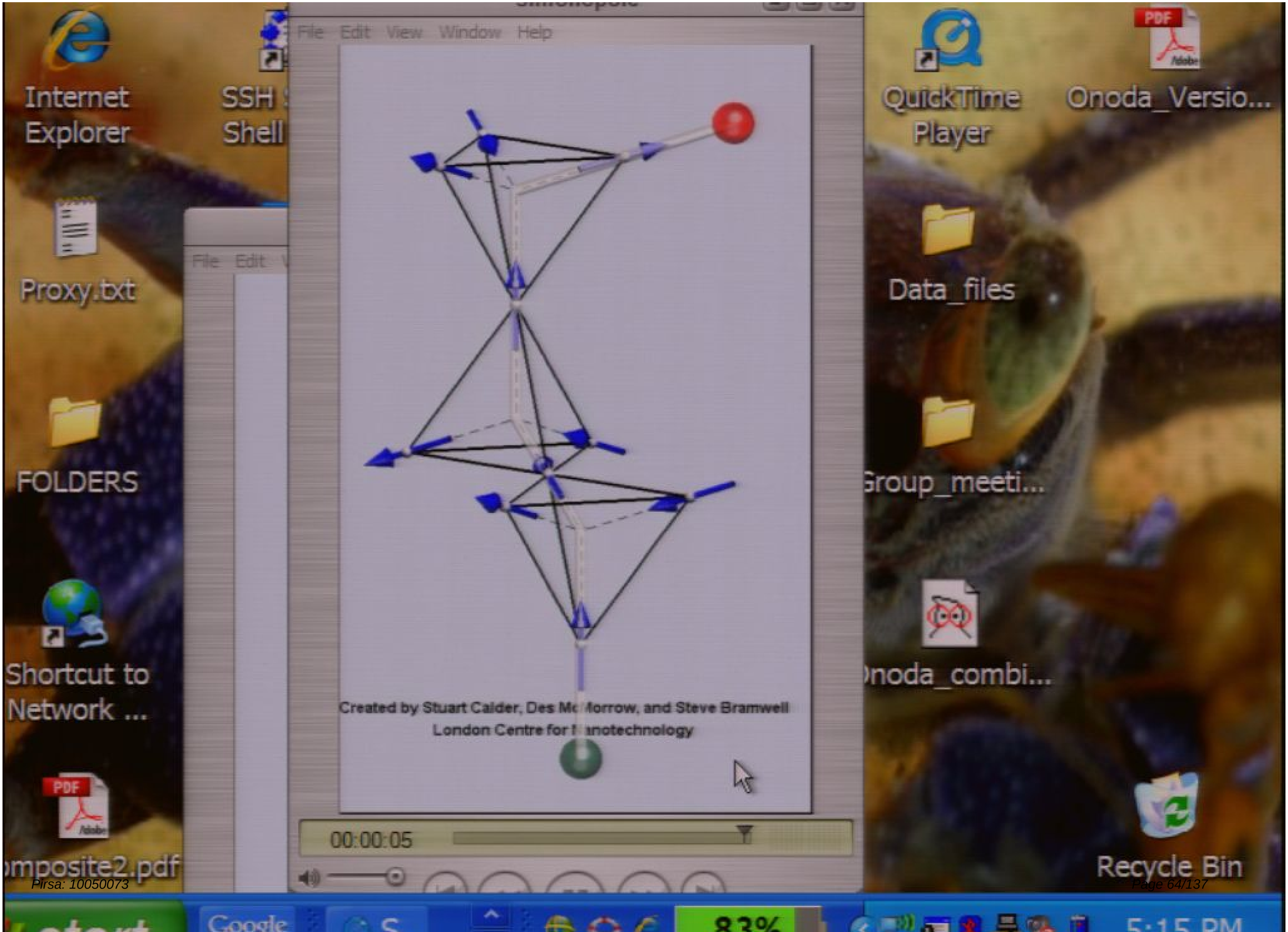
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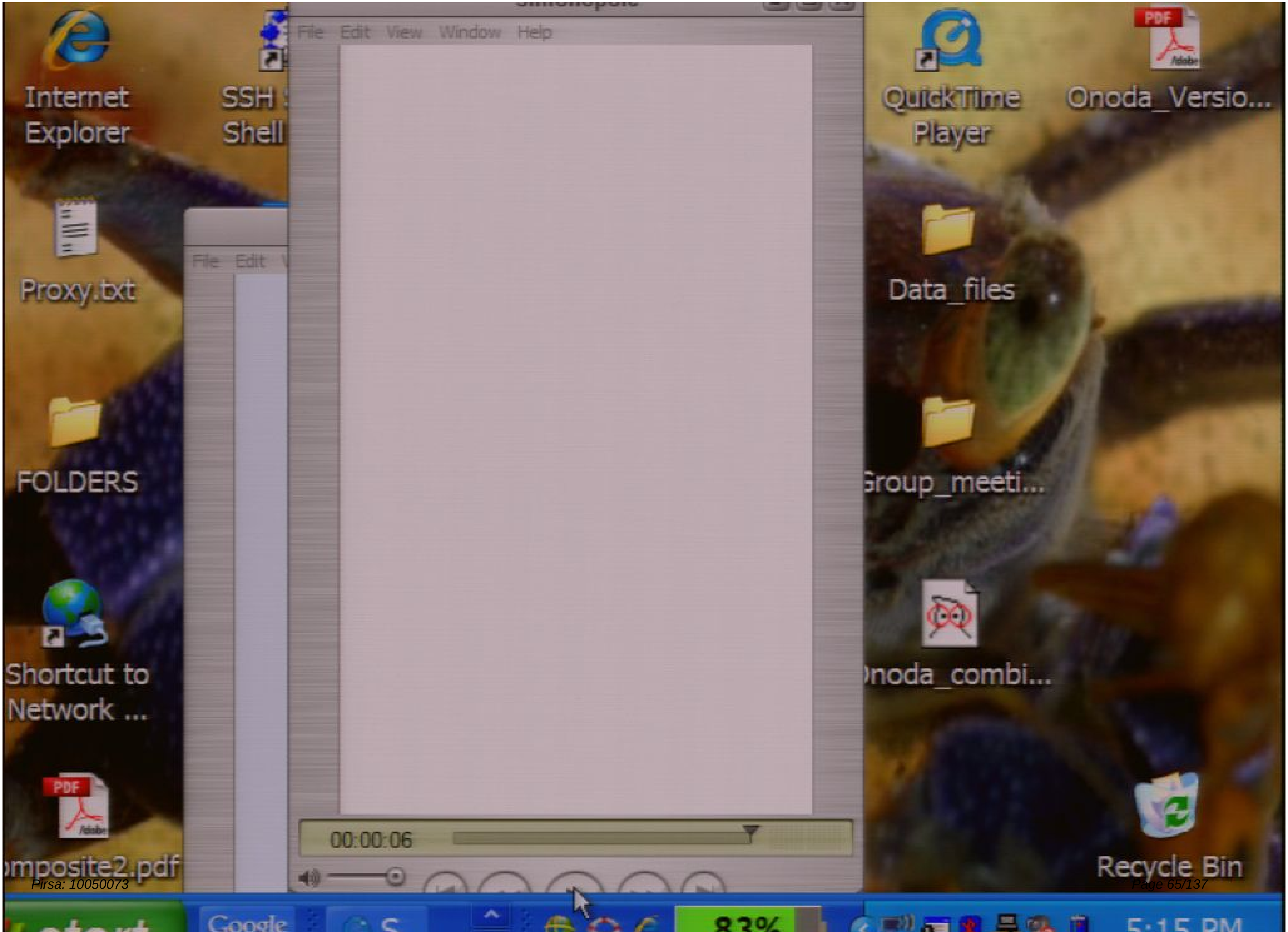
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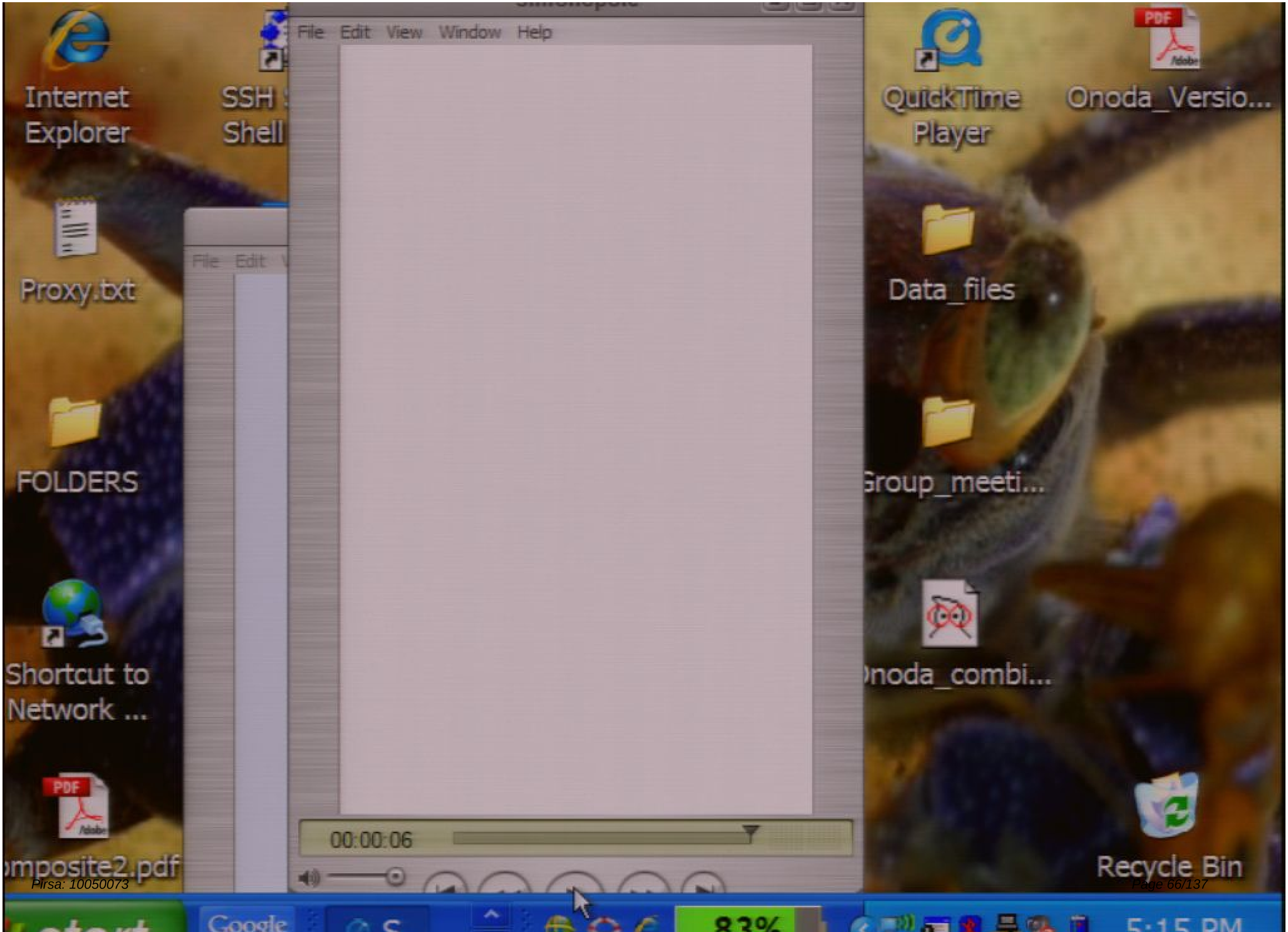
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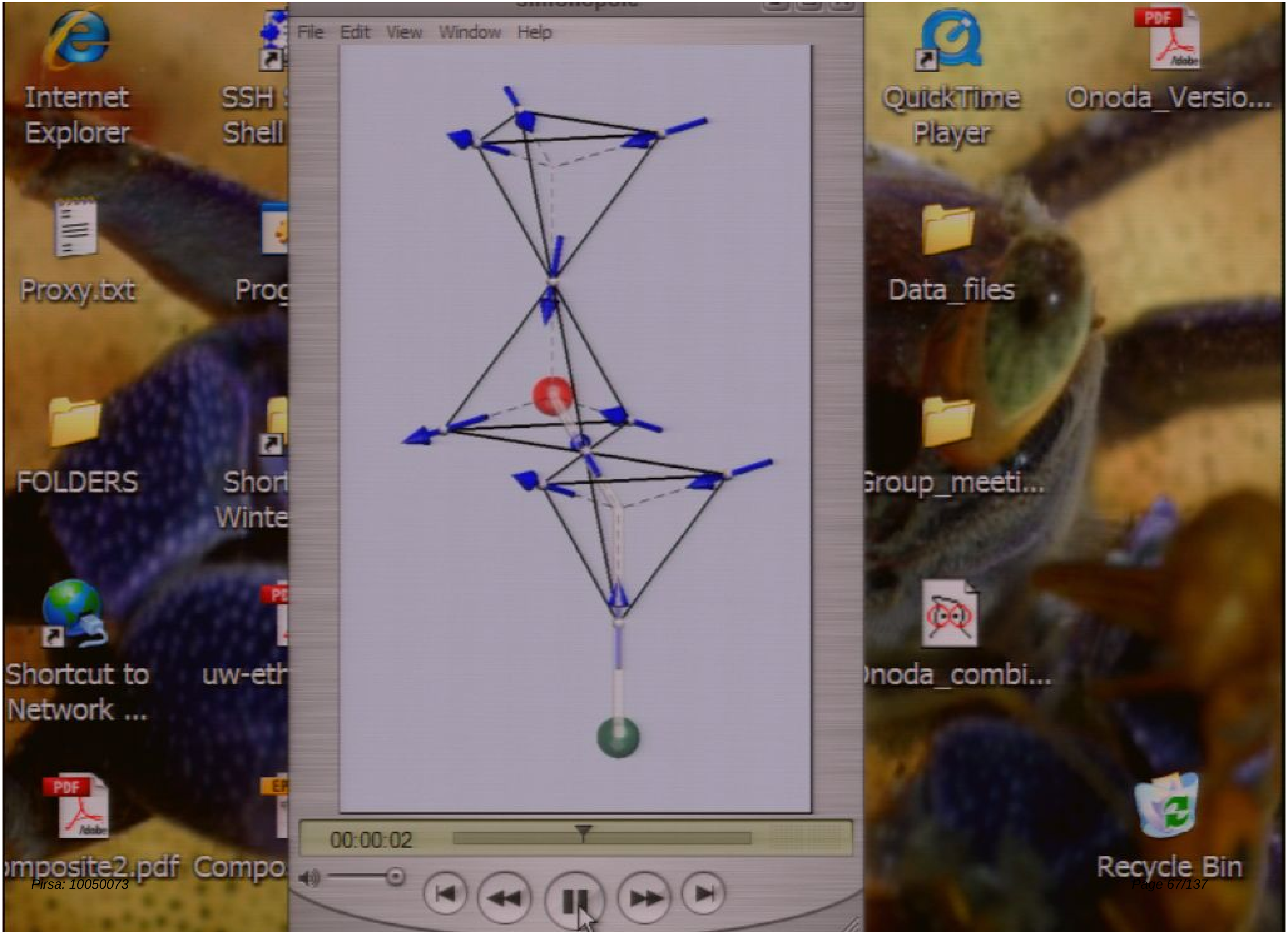
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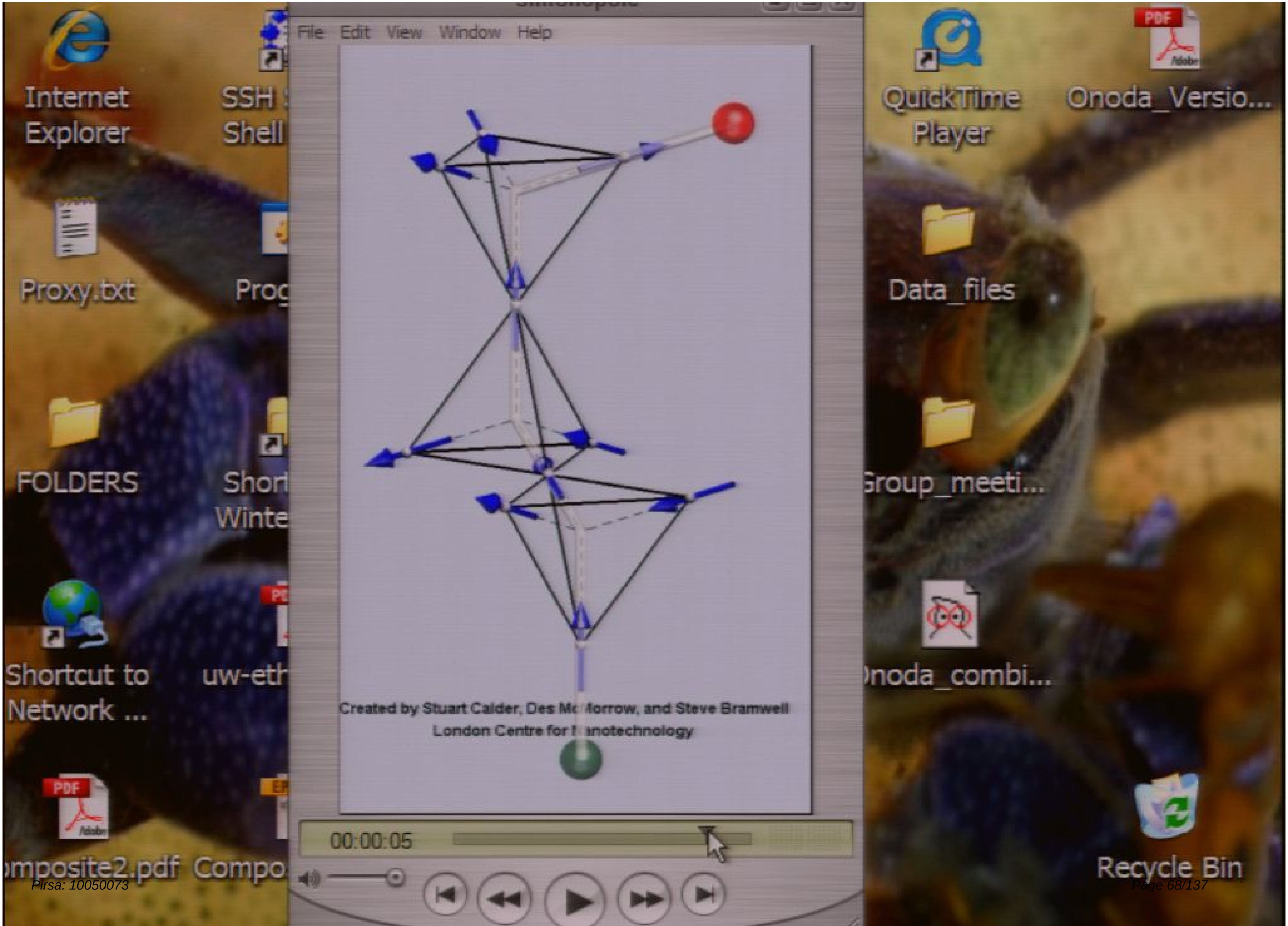
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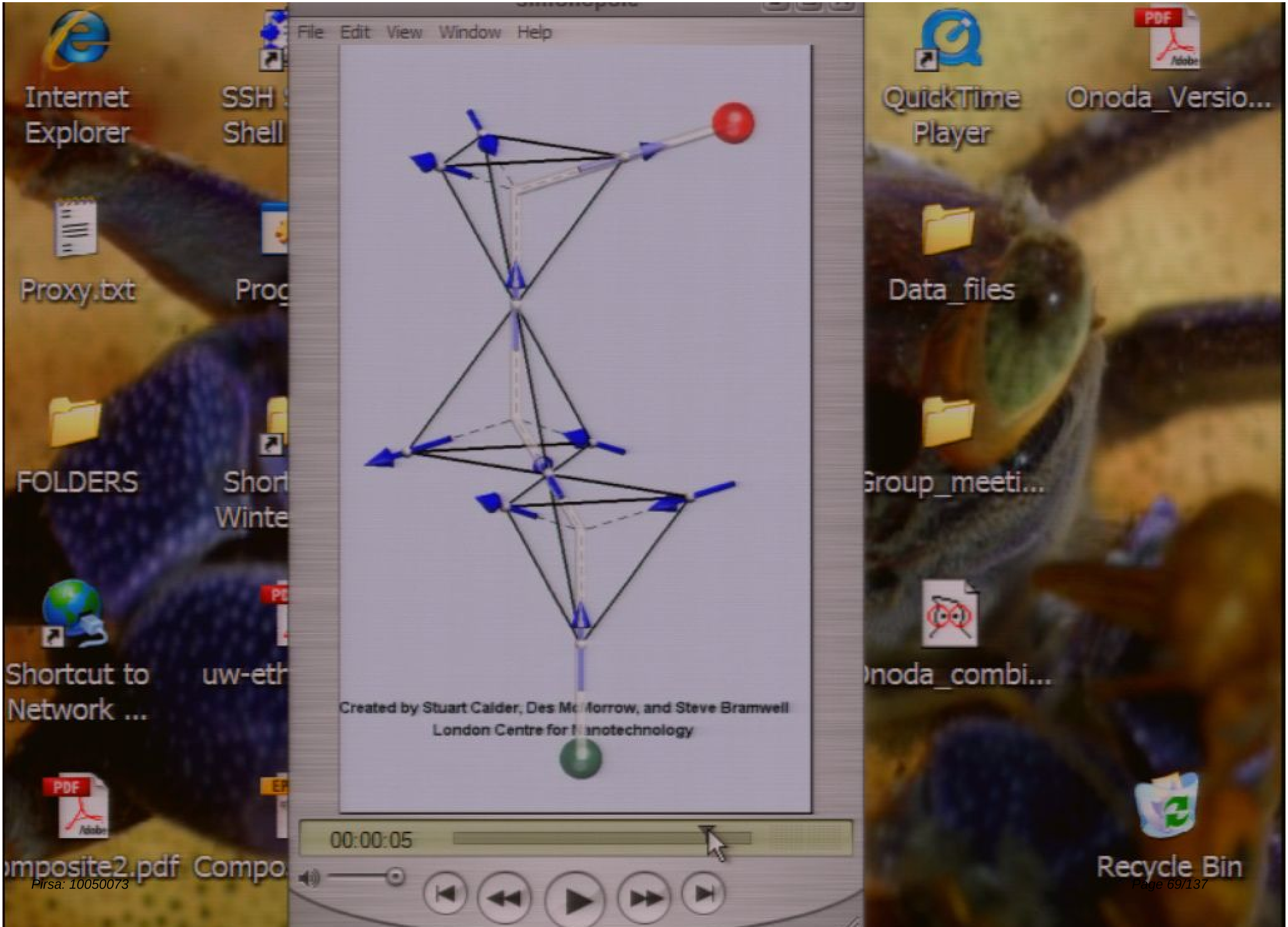
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Nature of the spin spin correlations

- Effective theory $$H_{\text{eff}} \sim \frac{\kappa}{2}\int d^3 r \left|\vec{P}\right|^2$$

- Since $\nabla \bullet \vec{P} = 0$ in absence of defects – one can introduce a vector potential such that $\vec{P} = \nabla \times \vec{A}$

$$\left\langle P_u(\vec{k}) P_v(\vec{k}) \right\rangle = \frac{1}{\kappa}\left(\delta_{uv} - \frac{k_u k_v}{k^2} \right)$$

- One can then use that to calculate the magnetic structure factor measured in a neutron experiment

C.L. Henley, arXiv:0912.4531

Nature of the spin spin correlations

- Effective theory $$H_{\text{eff}} \sim \frac{\kappa}{2}\int d^3 r \left|\vec{P}\right|^2$$

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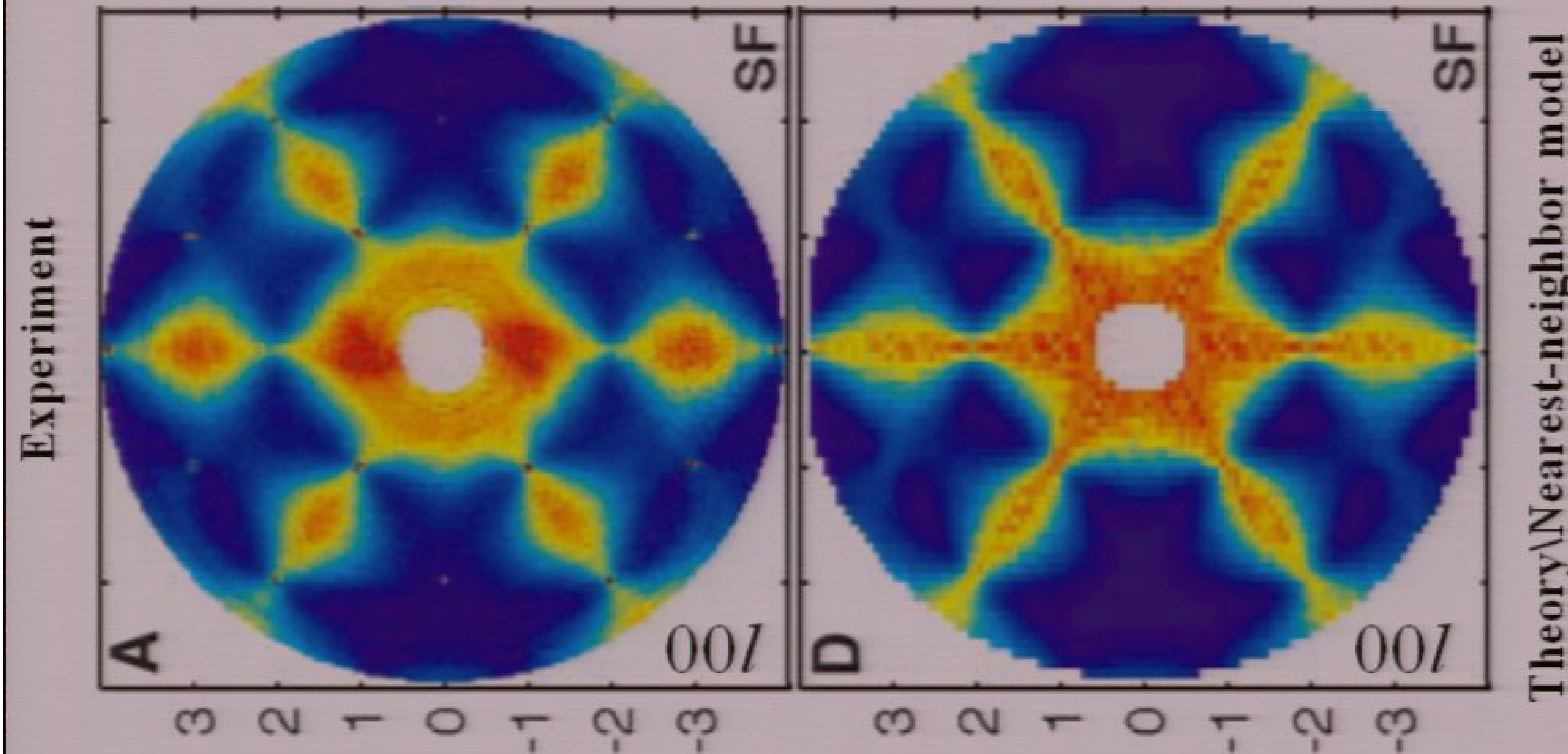
C.L. Henley arXiv:0912.4531

Singular correlations in spin ice state

- Because of the ice rule, hence the divergence free-condition of the field $\vec{P}$
- The spin-spin correlations in real-space decay as an effective dipolar type

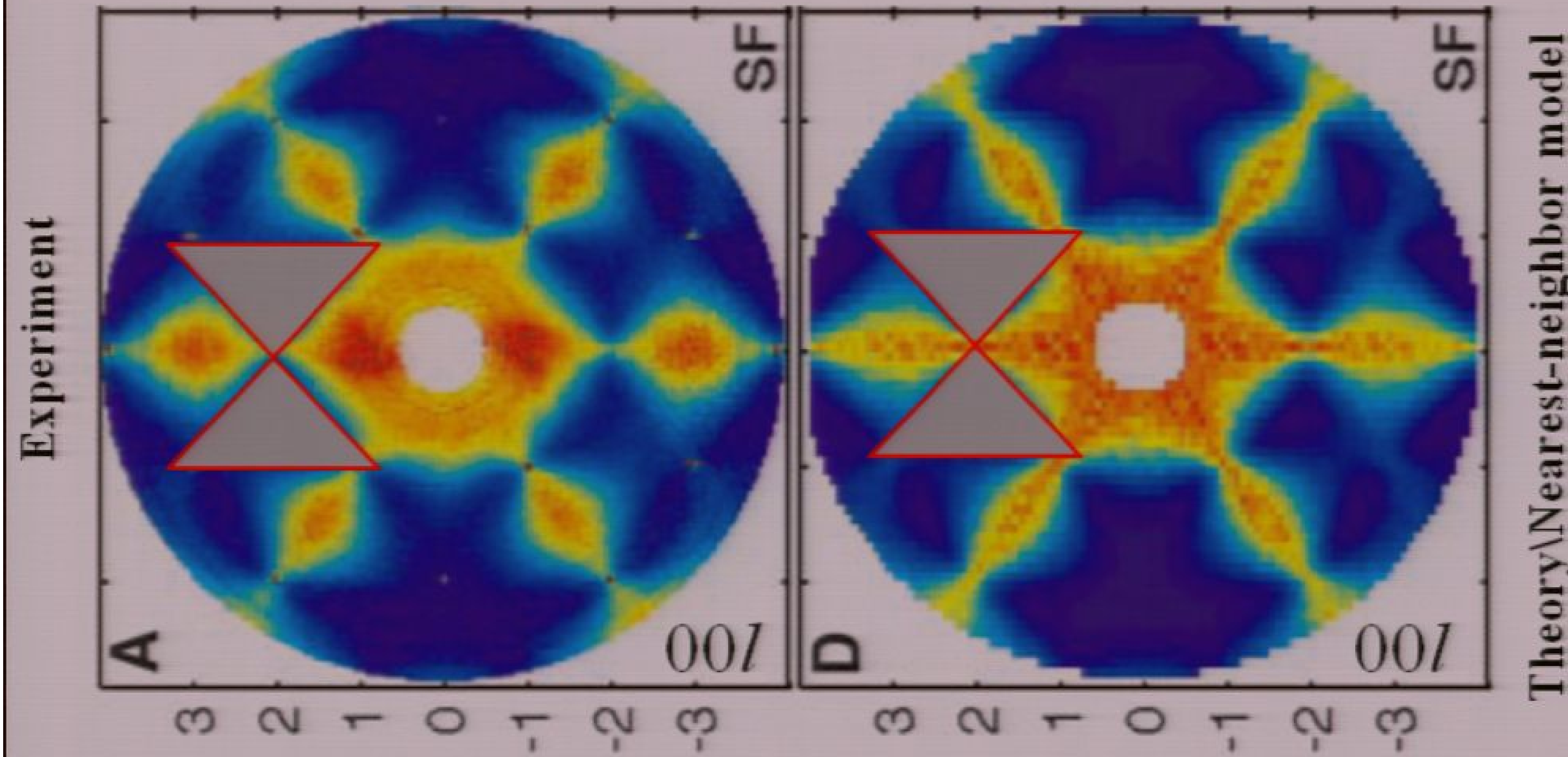
$$\left\langle P_u(\vec{r})\bullet P_v(\vec{r}\,')\right\rangle \sim \frac{r^2\delta_{uv}-3r_ur_v}{r^5}$$

- Very different than the exponential decay of the spin-spin correlations in a thermally disordered paramagnet
- As a result, the Fourier transform, hence the neutron scattering, show singular behaviors, "pinch points", at specific reciprocal lattice points.



$$S^{yy}(q_h, q_k, q_l) \propto \frac{q_{l-2}^2 + \xi_{\text{ice}}^{-2}}{q_{l-2}^2 + q_h^2 + q_k^2 + \xi_{\text{ice}}^{-2}}$$

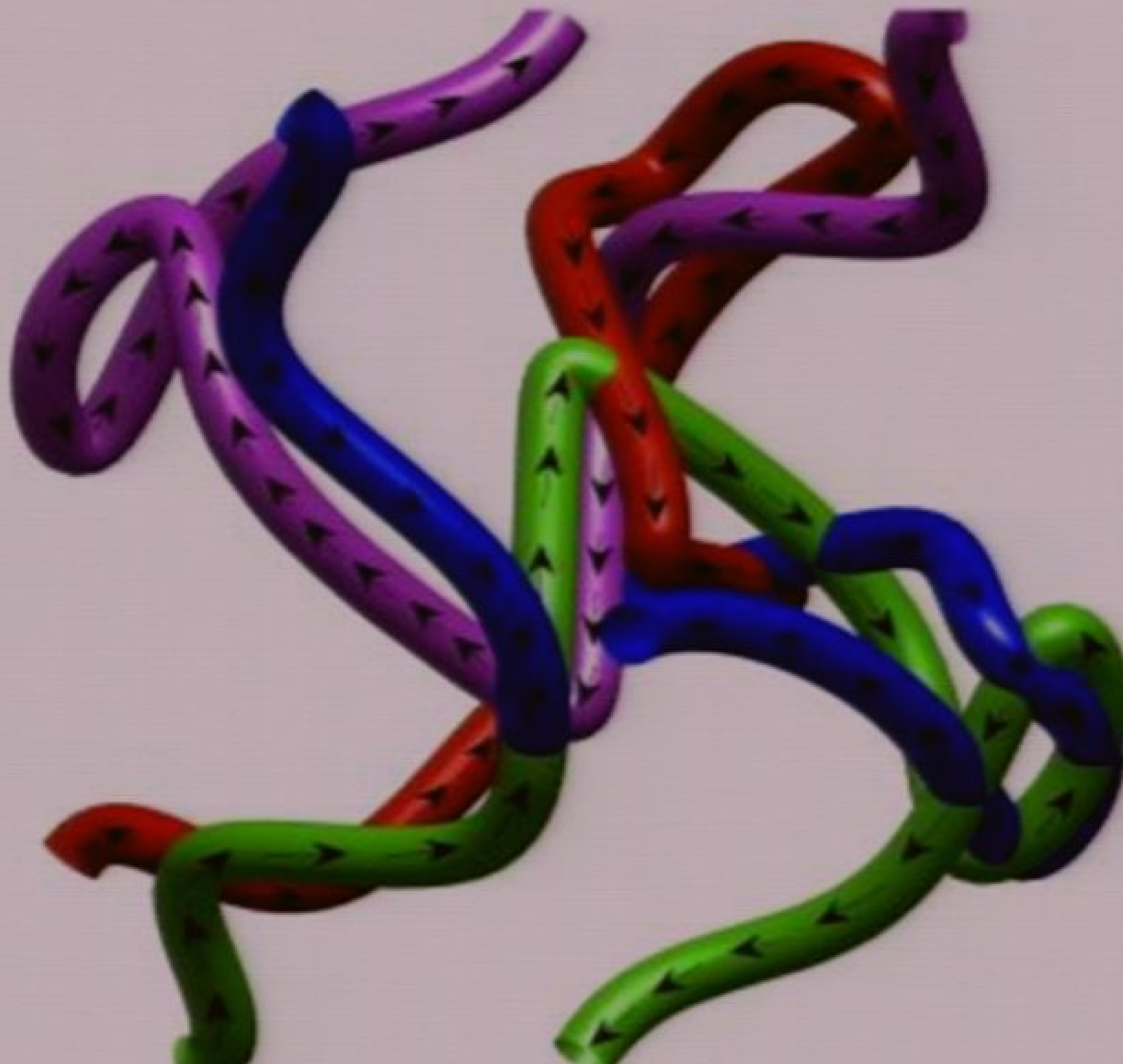
Fennell *et al.*, *Science* **326**, 415 (2009)



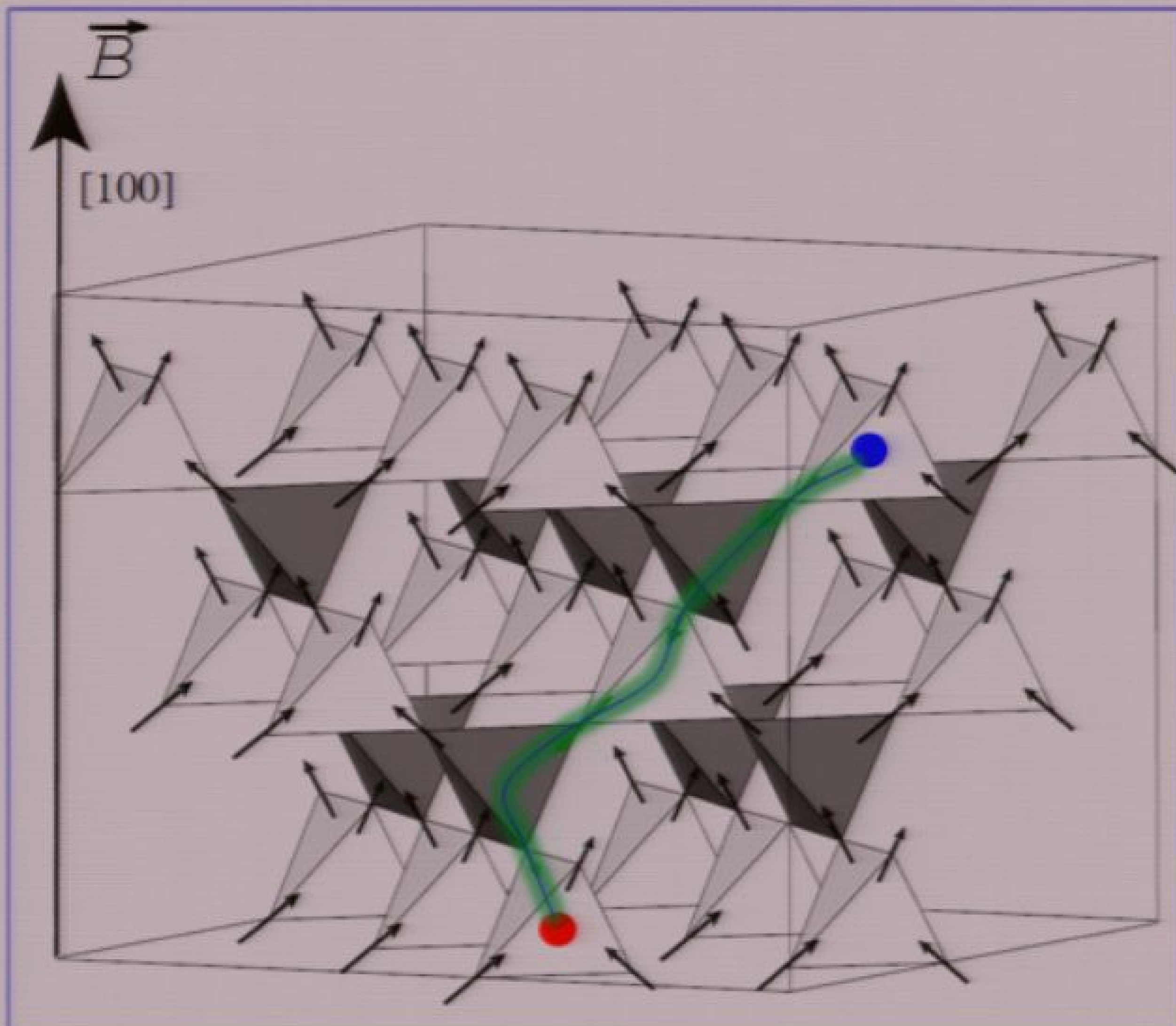
$$S^{yy}(q_h, q_k, q_l) \propto \frac{q_{l-2}^2 + \xi_{\text{ice}}^{-2}}{q_{l-2}^2 + q_h^2 + q_k^2 + \xi_{\text{ice}}^{-2}}$$

Fennell *et al.*, *Science* **326**, 415 (2009)

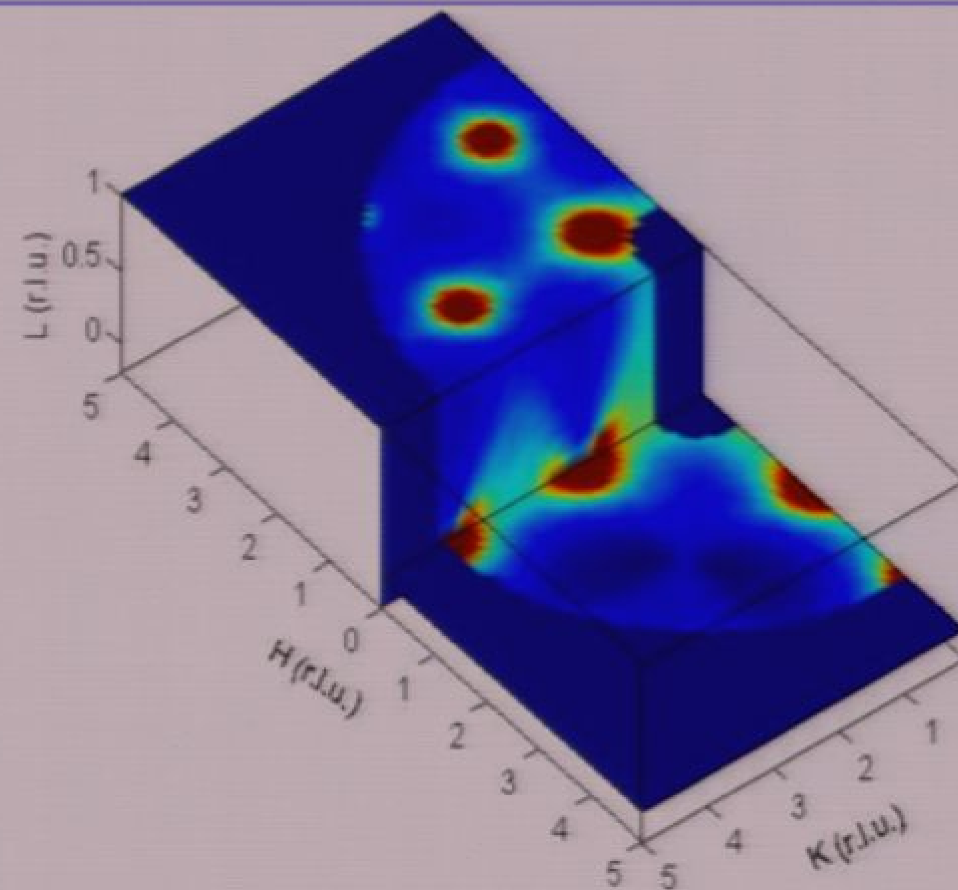
Dirac strings soup in zero a magnetic field



Oriented Dirac strings in a magnetic field

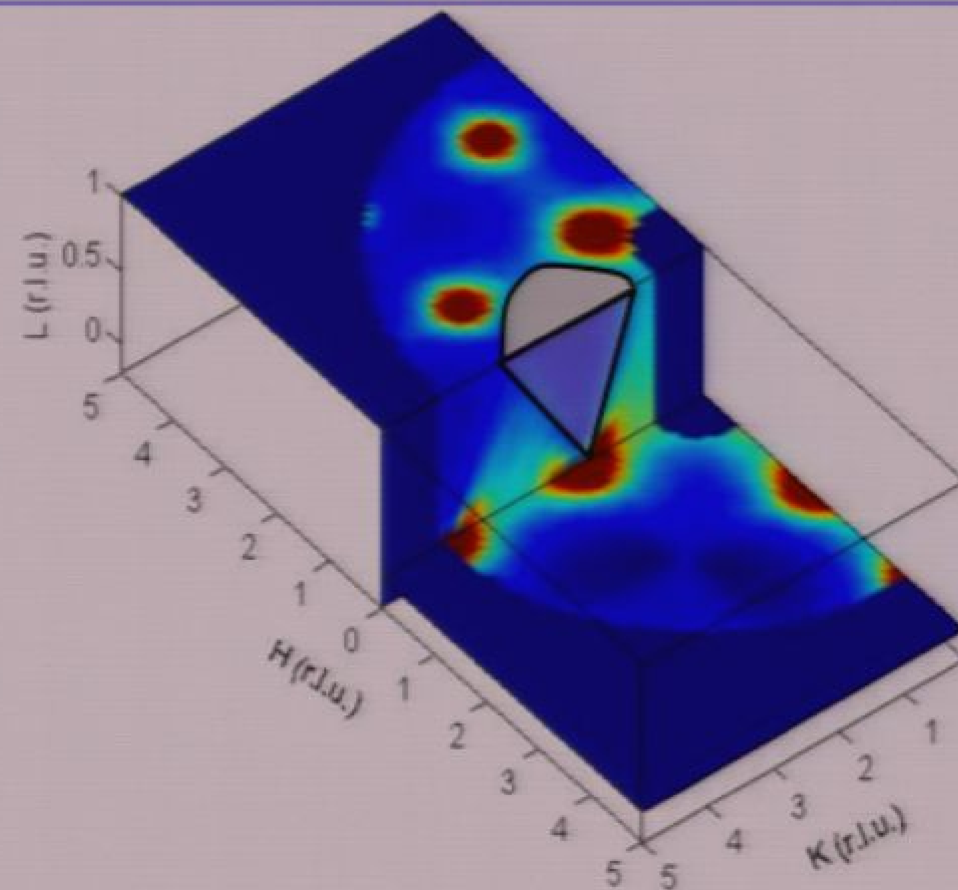


"Dirac strings" in a magnetic field



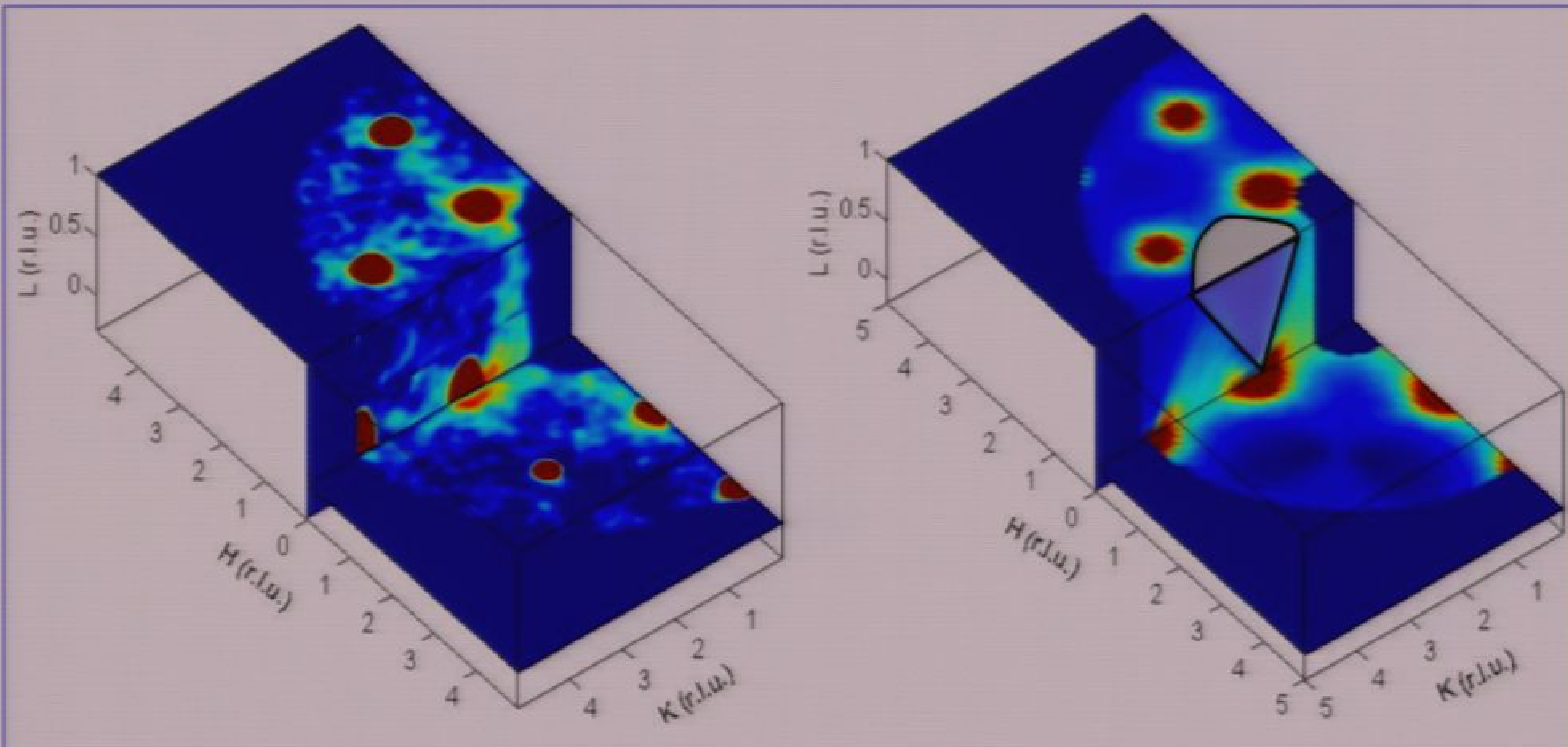
Morris *et al.*, *Science* **326**, 411 (2009)

“Dirac strings” in a magnetic field



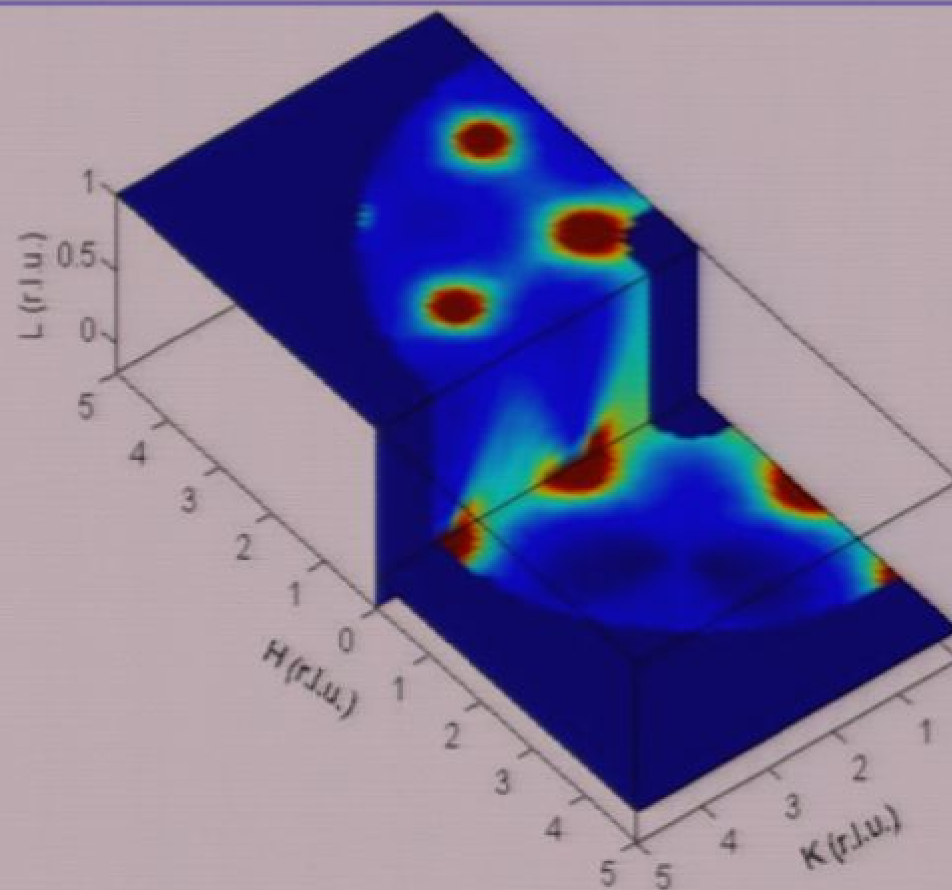
Morris *et al.*, *Science* **326**, 411 (2009)

"Dirac strings" in a magnetic field



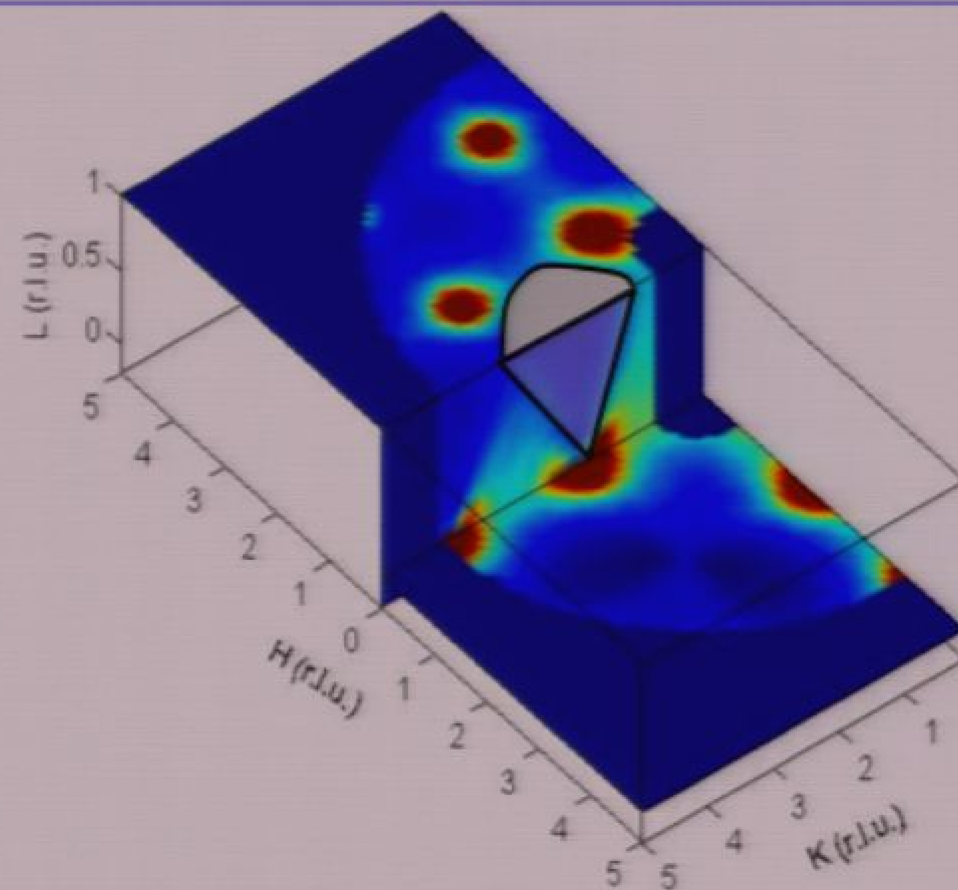
Morris *et al.*, *Science* ***326***, 411 (2009)

“Dirac strings” in a magnetic field



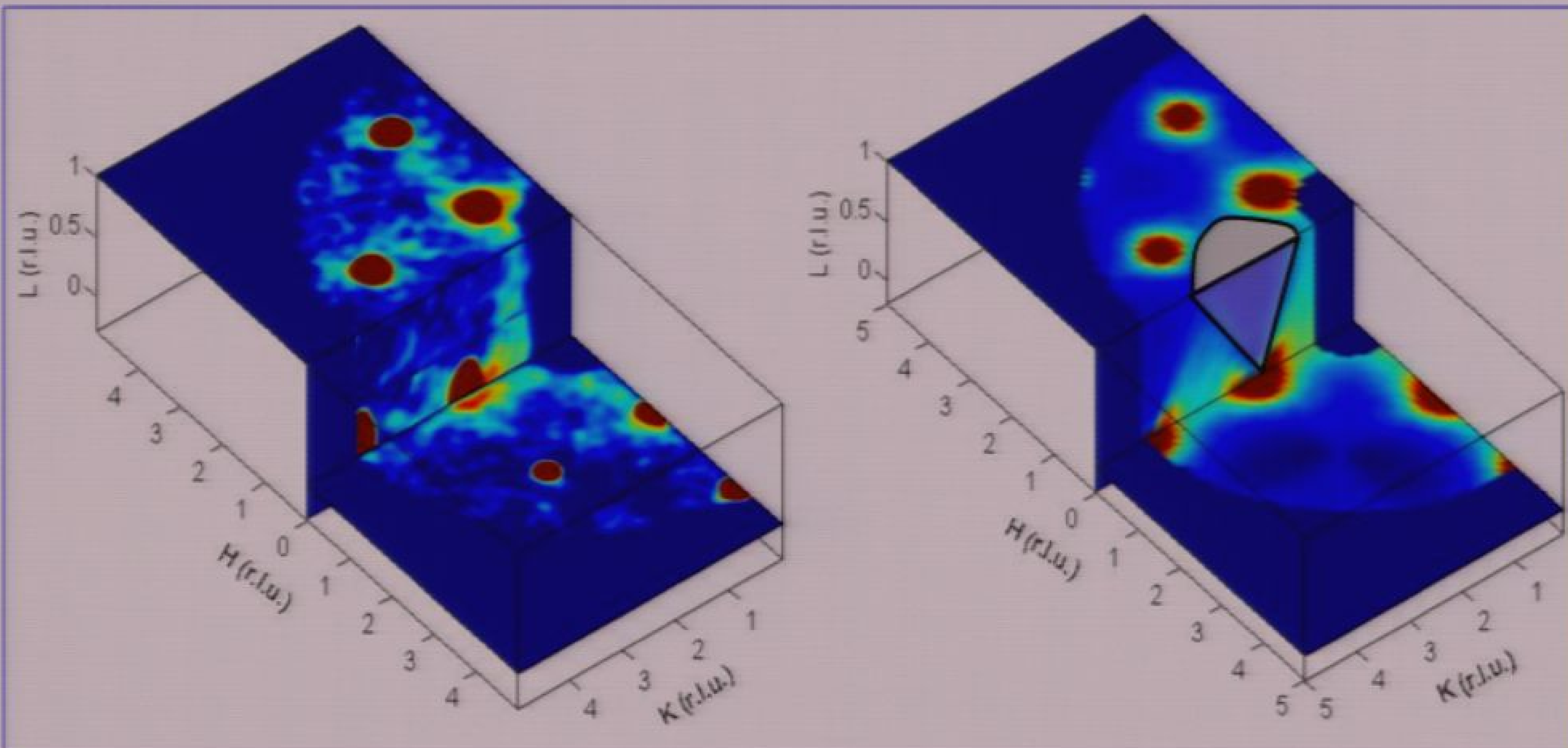
Morris *et al.*, *Science* ***326***, 411 (2009)

“Dirac strings” in a magnetic field



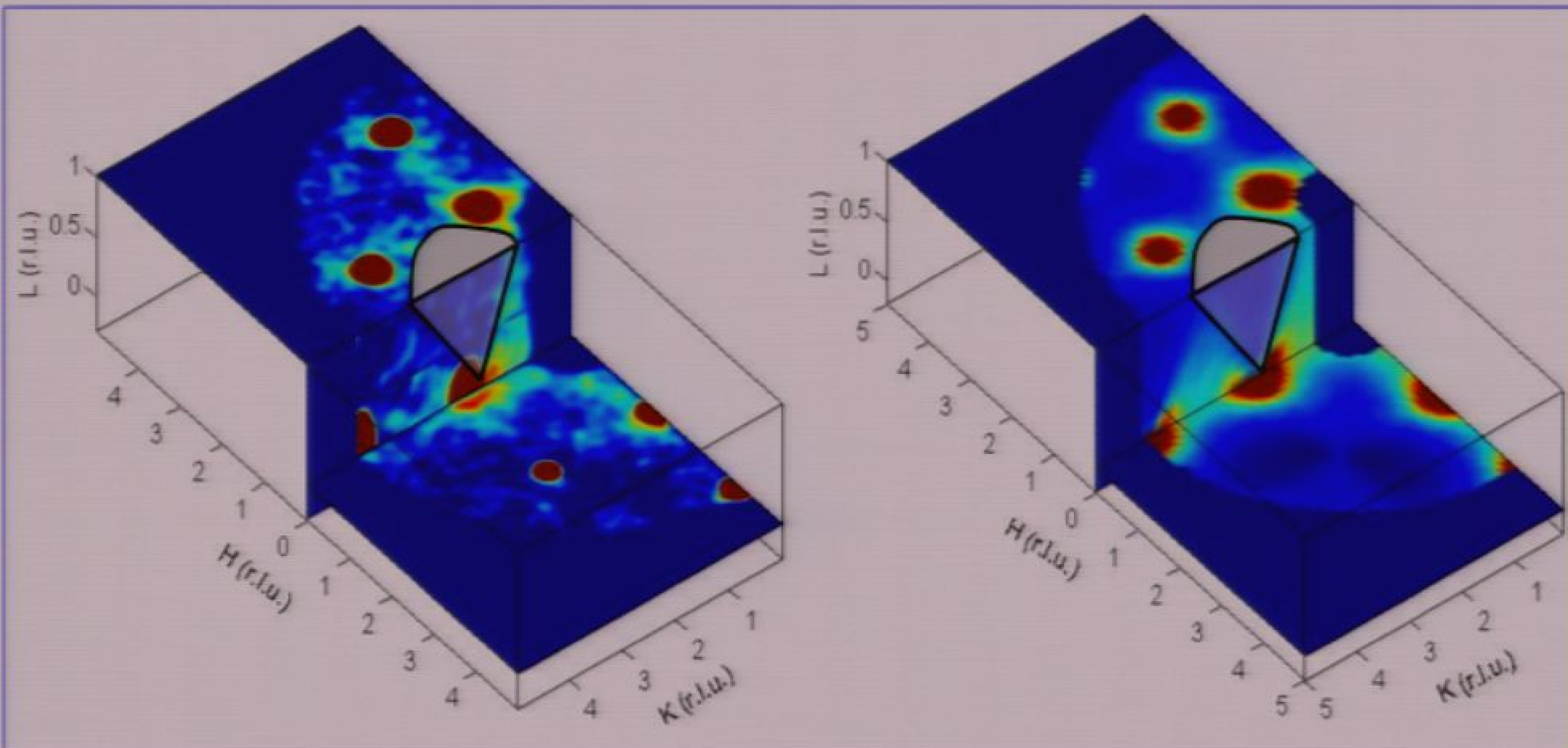
Morris *et al.*, *Science* **326**, 411 (2009)

“Dirac strings” in a magnetic field



Morris *et al.*, *Science* **326**, 411 (2009)

"Dirac strings" in a magnetic field



Morris *et al.*, *Science* **326**, 411 (2009)

nature

NATURE **461**, 956 (2009)

LETTERS

Measurement of the charge and current of magnetic monopoles in spin ice

S. T. Bramwell[1]*, S. R. Giblin[2]*, S. Calder[1], R. Aldus[1], D. Prabhakaran[3] & T. Fennell[4]

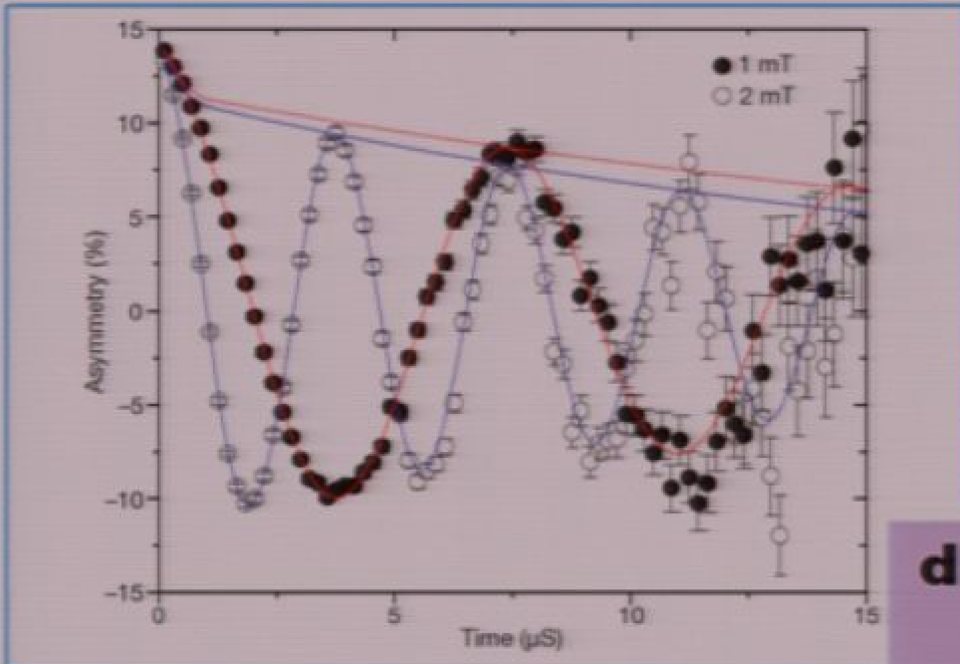
Onsager's 1934 theory of Wien's 2nd effect (dissociation rate, *K*, of water subject to an electric field)

$$2H_2O = [H_3O^+OH^-] = H_3O^+ + OH^-$$

$$e \rightarrow Q,\ E \rightarrow B,\ \varepsilon_0 \rightarrow \mu_0^{-1}$$

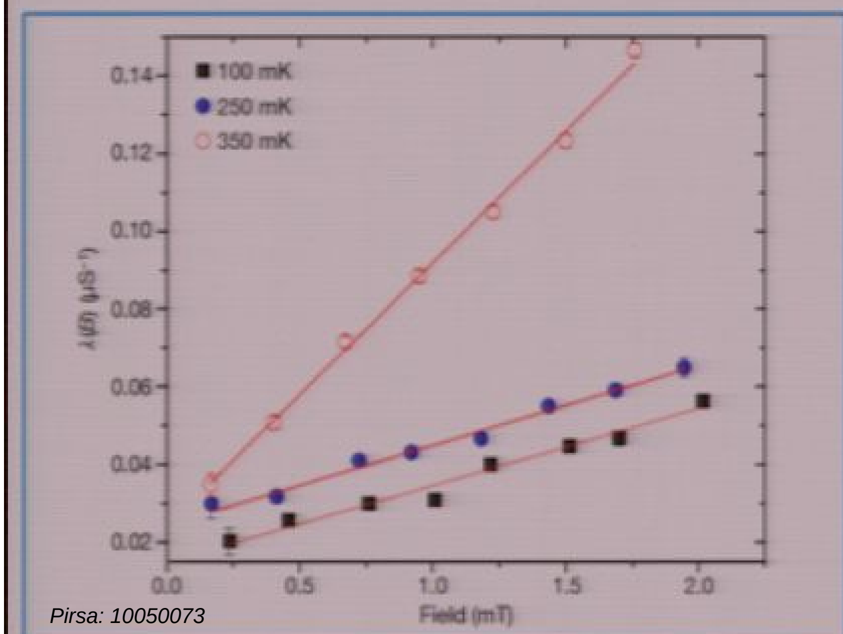
$$K(B) = K(0)\left(1 + b + \frac{b^2}{3}\dots\right)$$

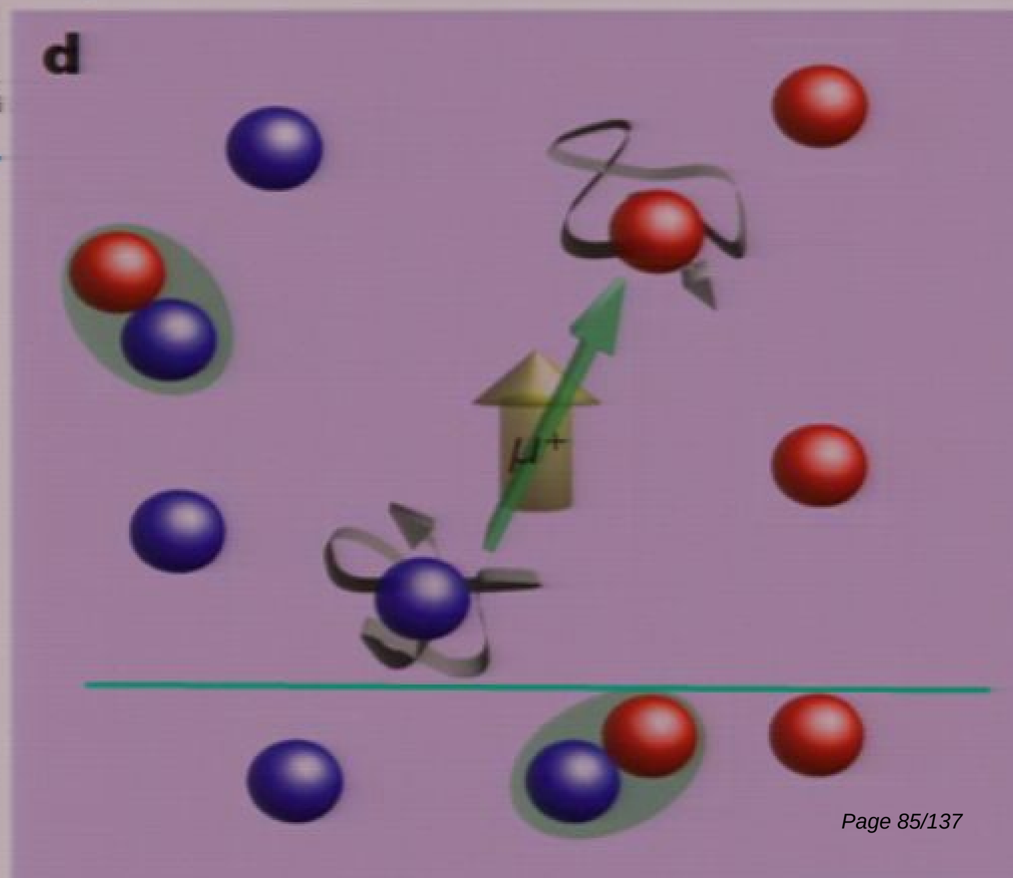
$$b = \frac{\mu_0 Q^3 B}{8\pi k^2 T^2}$$

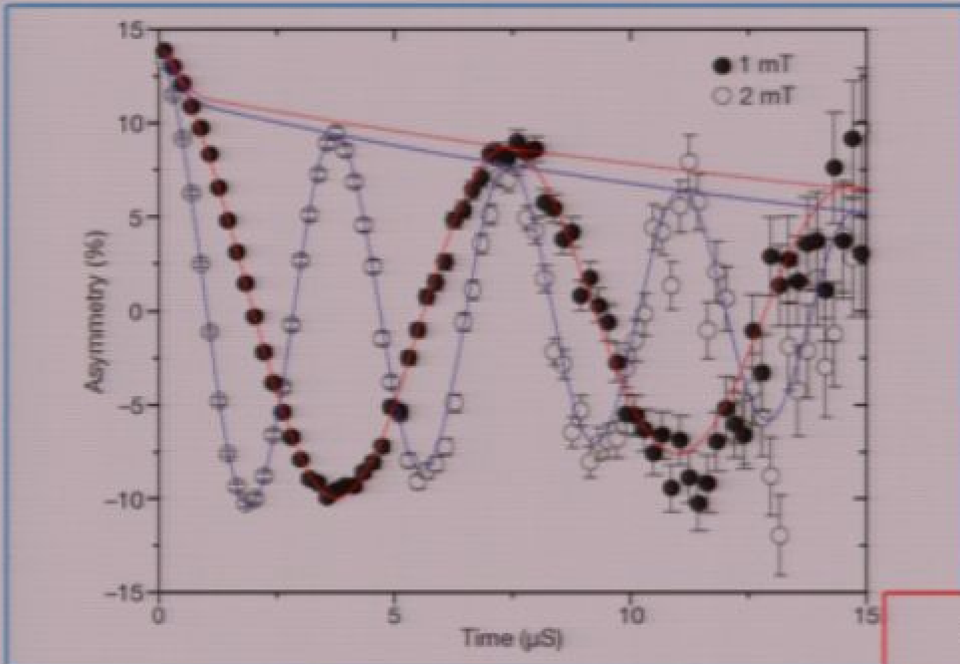


$$\frac{v_\mu(B)}{v_\mu(0)} = \frac{\kappa(B)}{\kappa(0)} = 1 + \frac{b}{2}$$

$$b = \frac{\mu_0 Q^3 B}{8\pi k^2 T^2}$$







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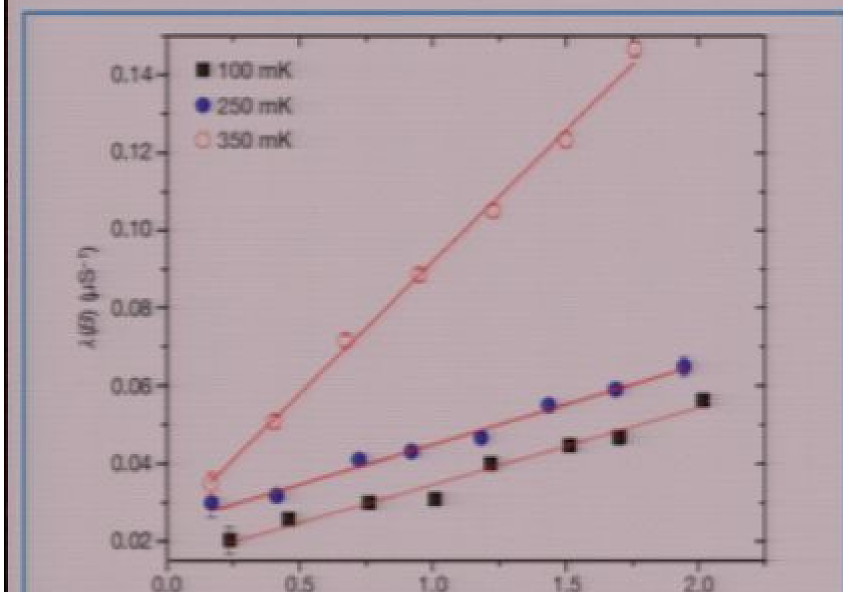
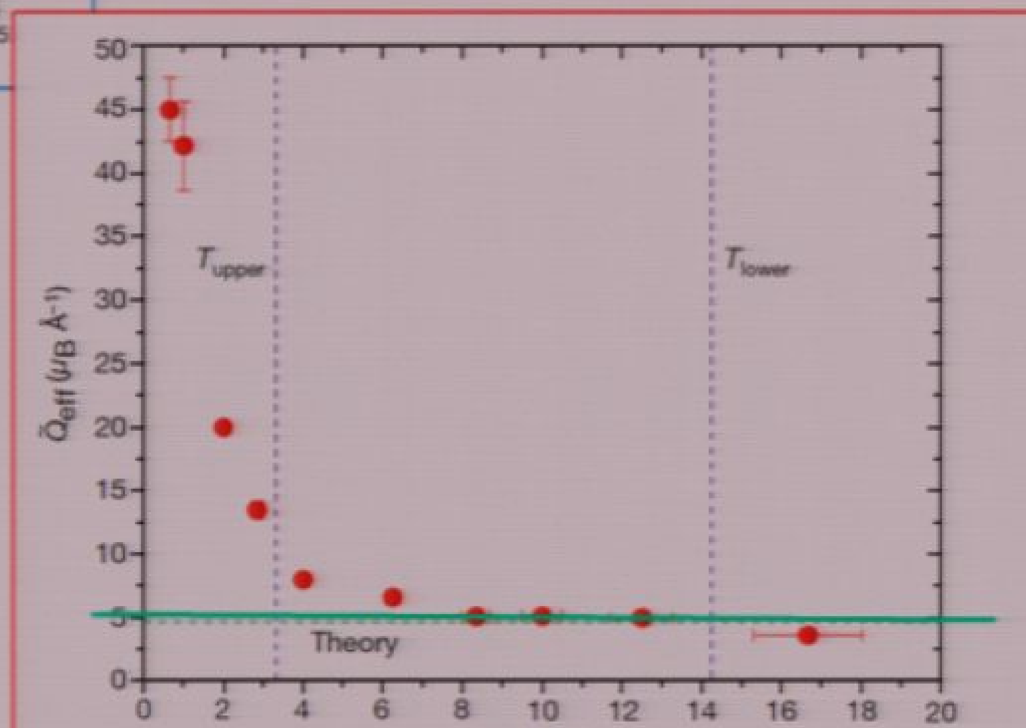




"Conclusion" about Monopoles in Spin ice

- Excitations in spin ices consists of deconfined monopole-like topological defects
- These have been recently observed and reported in 2 neutron scattering papers in *Science* and 1 muon spin relaxation paper in *Nature (Oct. 2009)*.
- There is currently efforts in understanding the role of these objects on the spin dynamics in spin ice.

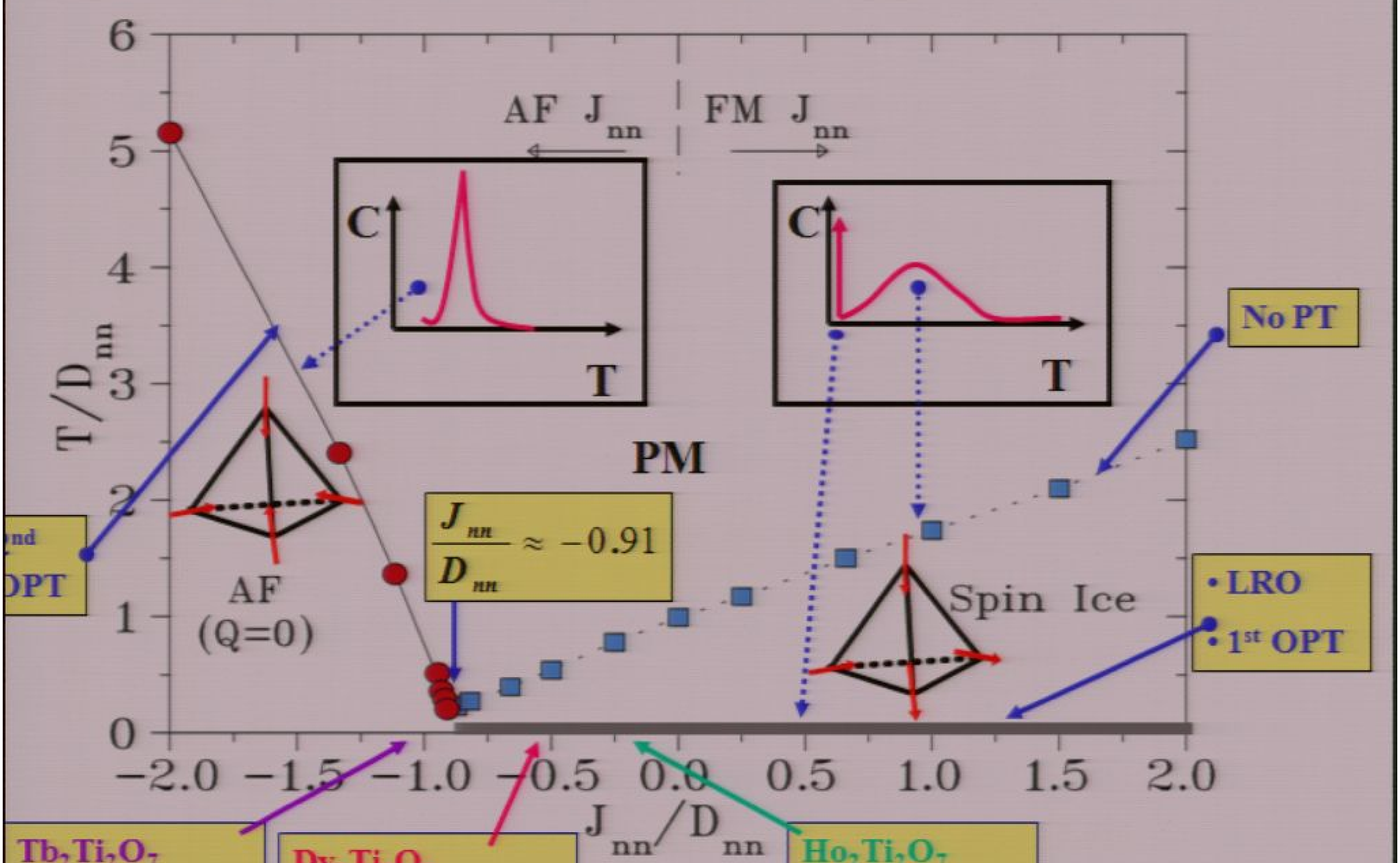
  Jaubert, L. D. C. & Holdsworth, P. C. W. Signature of magnetic monopole and Dirac string dynamics in spin ice. *Nature Phys.* 5, 258–261 (2009).

- There are bound to be more interesting effects tied to monopoles and "Dirac strings" in spin ice to be reported over the next couple of years.

Outline

1. **Introduction – a review of spin ice physics**
   - *Frustrated ferromagnet & ice rules*
   - *extensive low-temperature entropy*
   - *role of dipolar interactions*
2. **Spin ice – recent developments**
   - *Coulomb phase and divergence free field*
   - *Spin-spin correlations*
   - *Excitations in the Coulomb phase and monopoles*
   - *Magnetic-field induced dissociation of ice rules*
3. **Spin liquid physics of $Tb_2Ti_2O_7$**
   - *Corrections to Ising model*
   - *"Quantum spin ice"*
4. **Conclusion**

Monte Carlo Phase Diagram of the Dipolar Spin Ice Model



$Tb_2Ti_2O_7$

$J_{nn}/D_{nn} \approx -1.1$

$Dy_2Ti_2O_7$

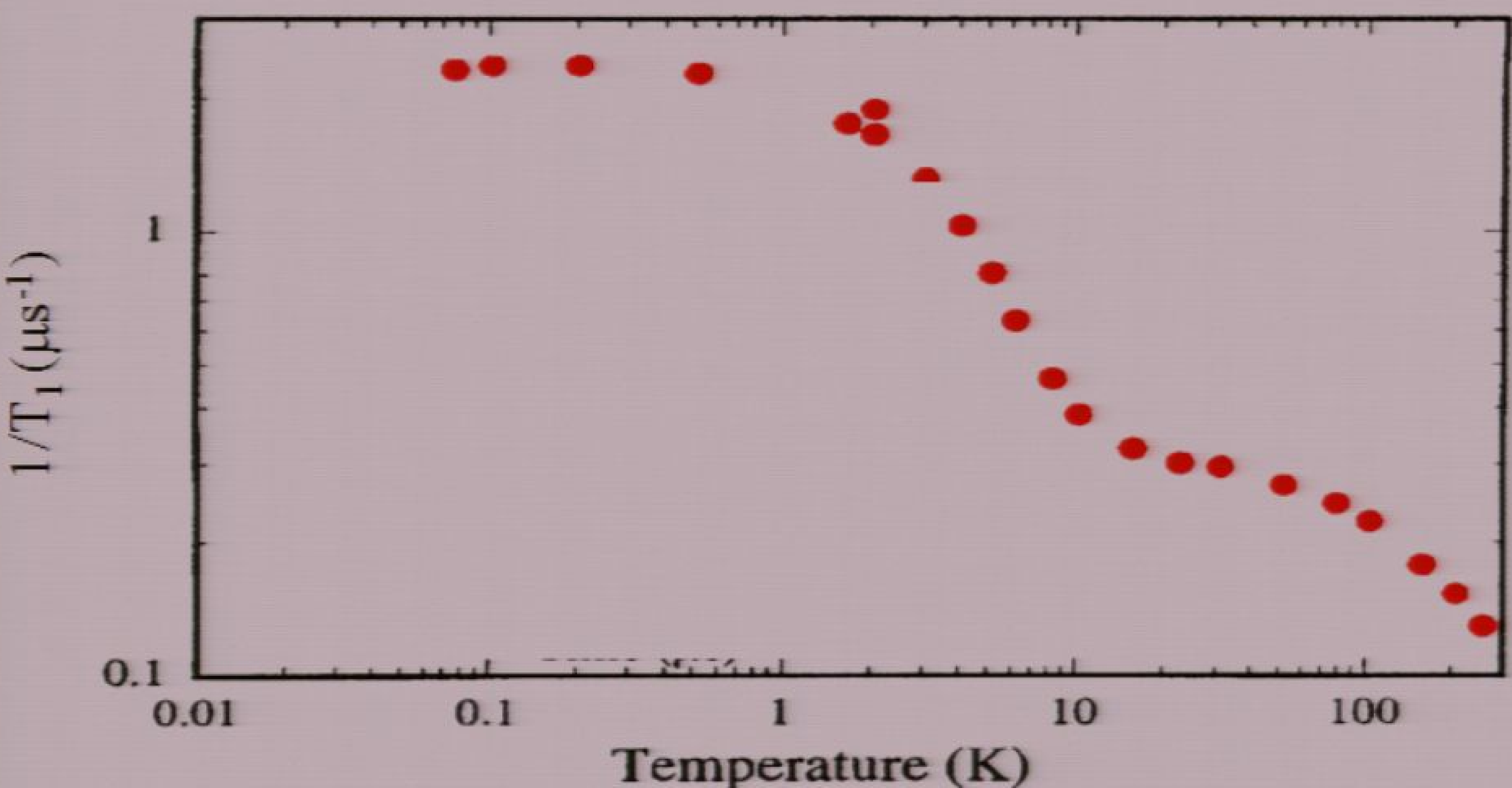
$J_{nn}/D_{nn} \approx -0.52$

$Ho_2Ti_2O_7$

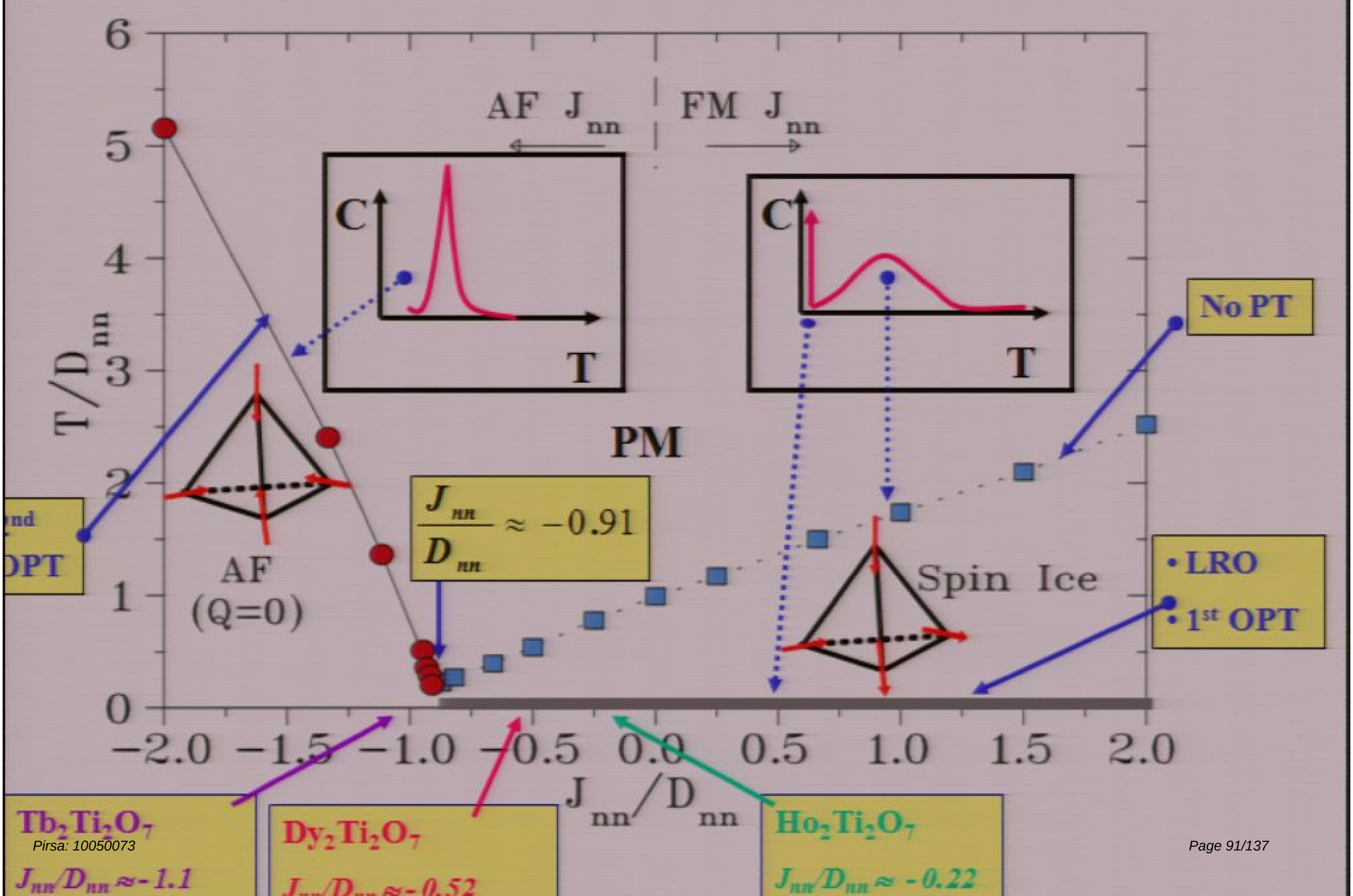
$J_{nn}/D_{nn} \approx -0.22$

Muon Spin Relaxation Study of $Tb_2Ti_2O_7$:

No sharp peak in the muon relaxation rate that would indicate a transition (or a "spin freezing") as a function of temperature from 100K down to 20 mK!!!



Monte Carlo Phase Diagram of the Dipolar Spin Ice Model



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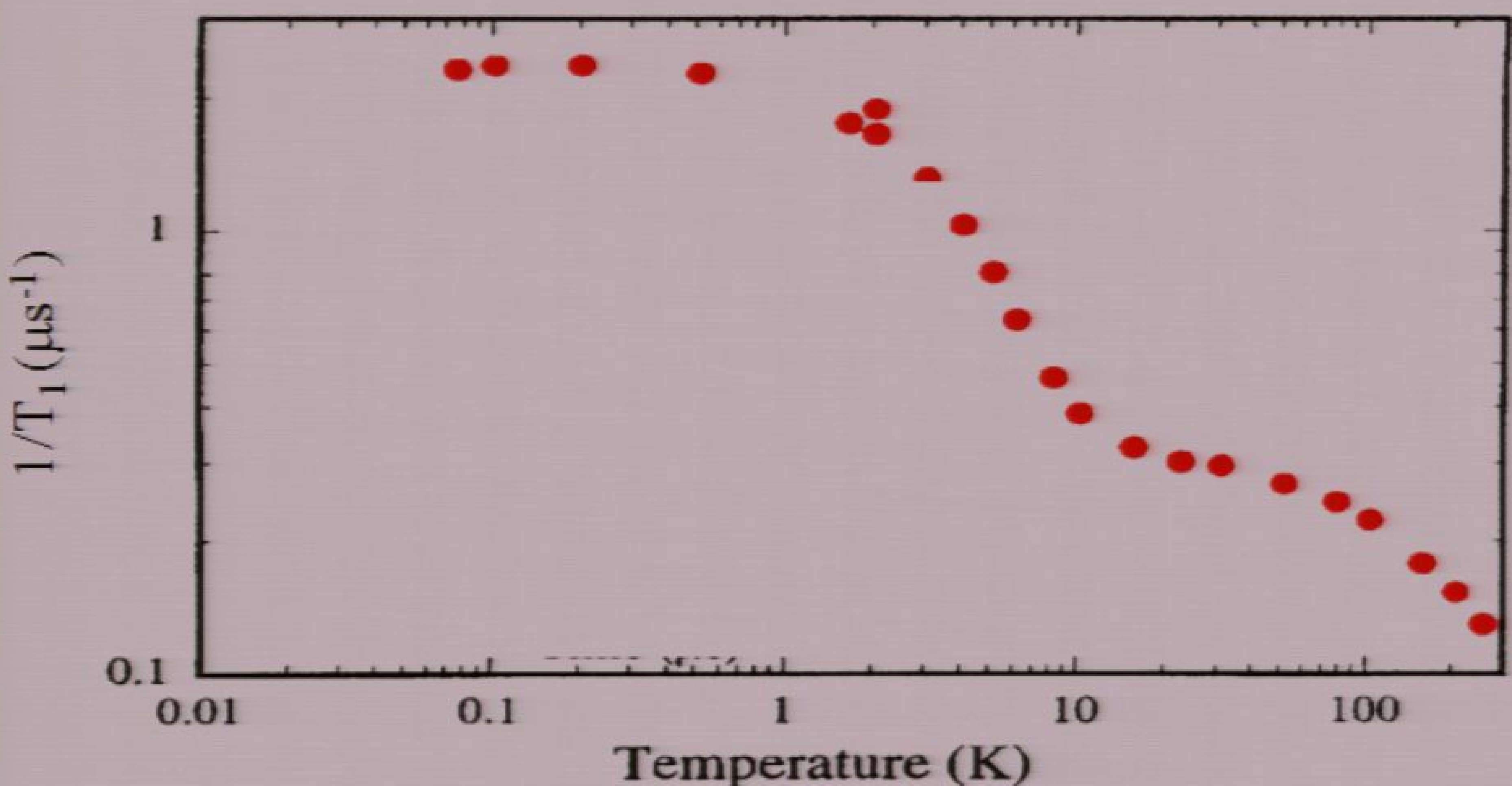

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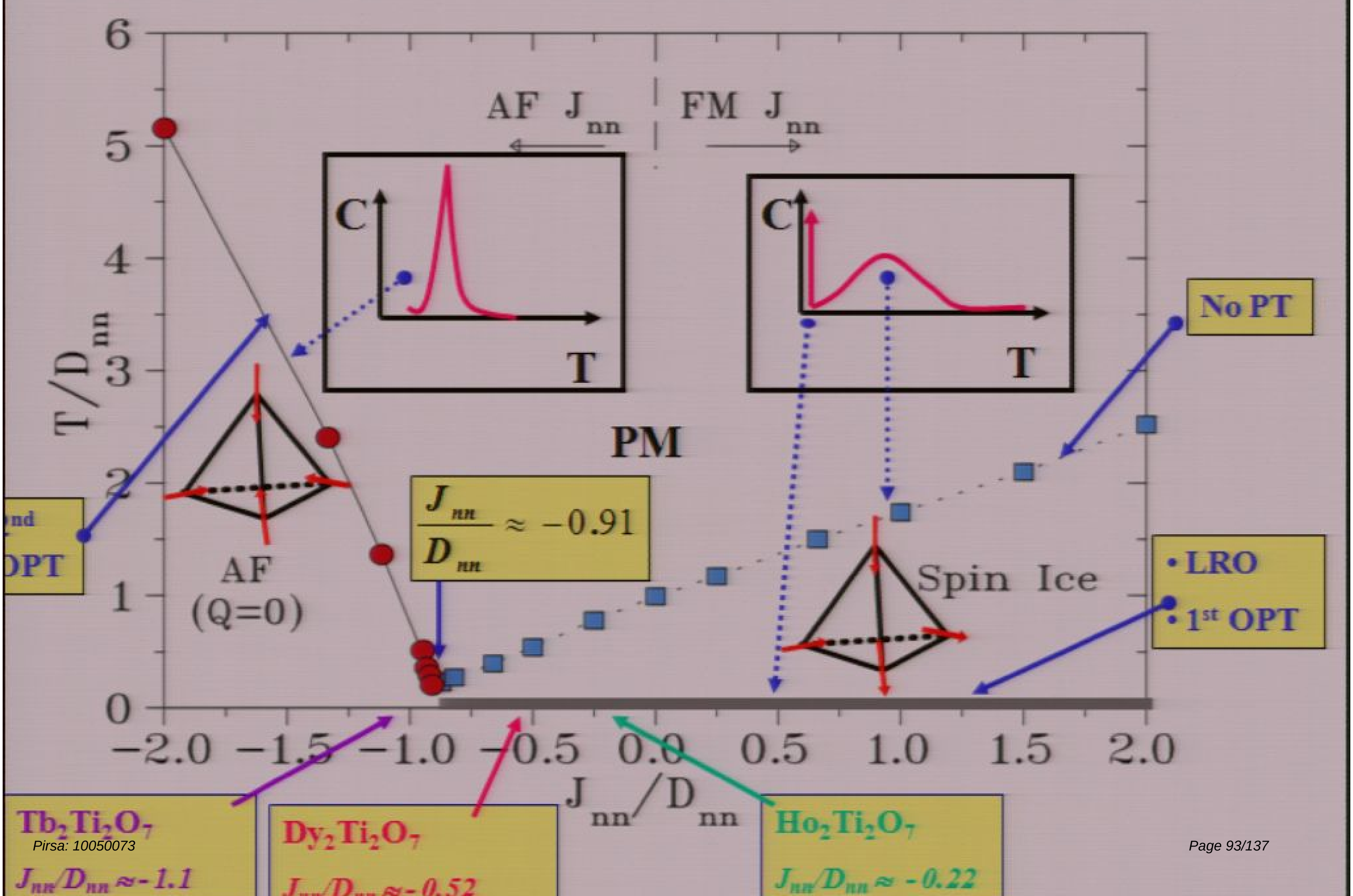

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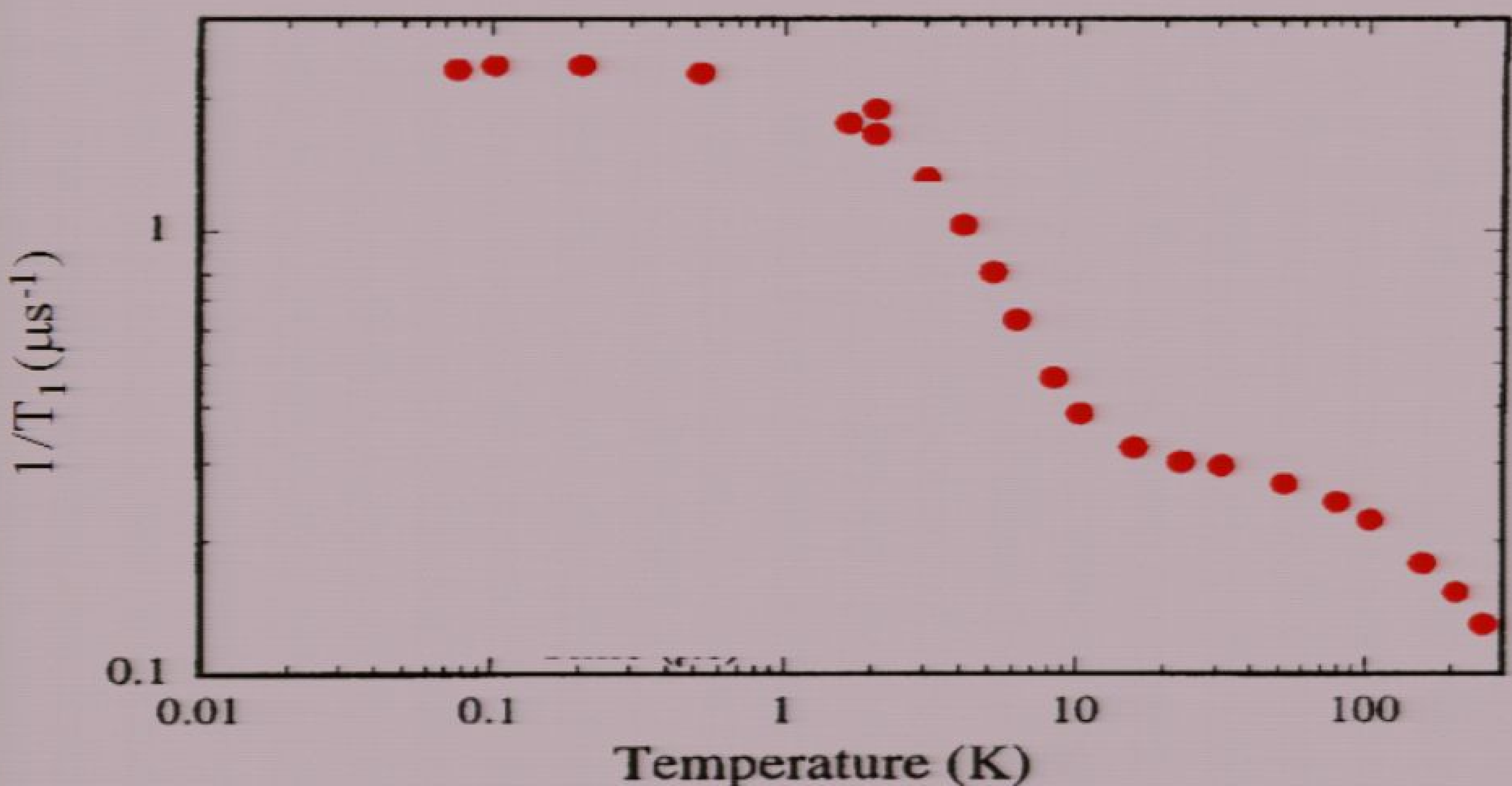
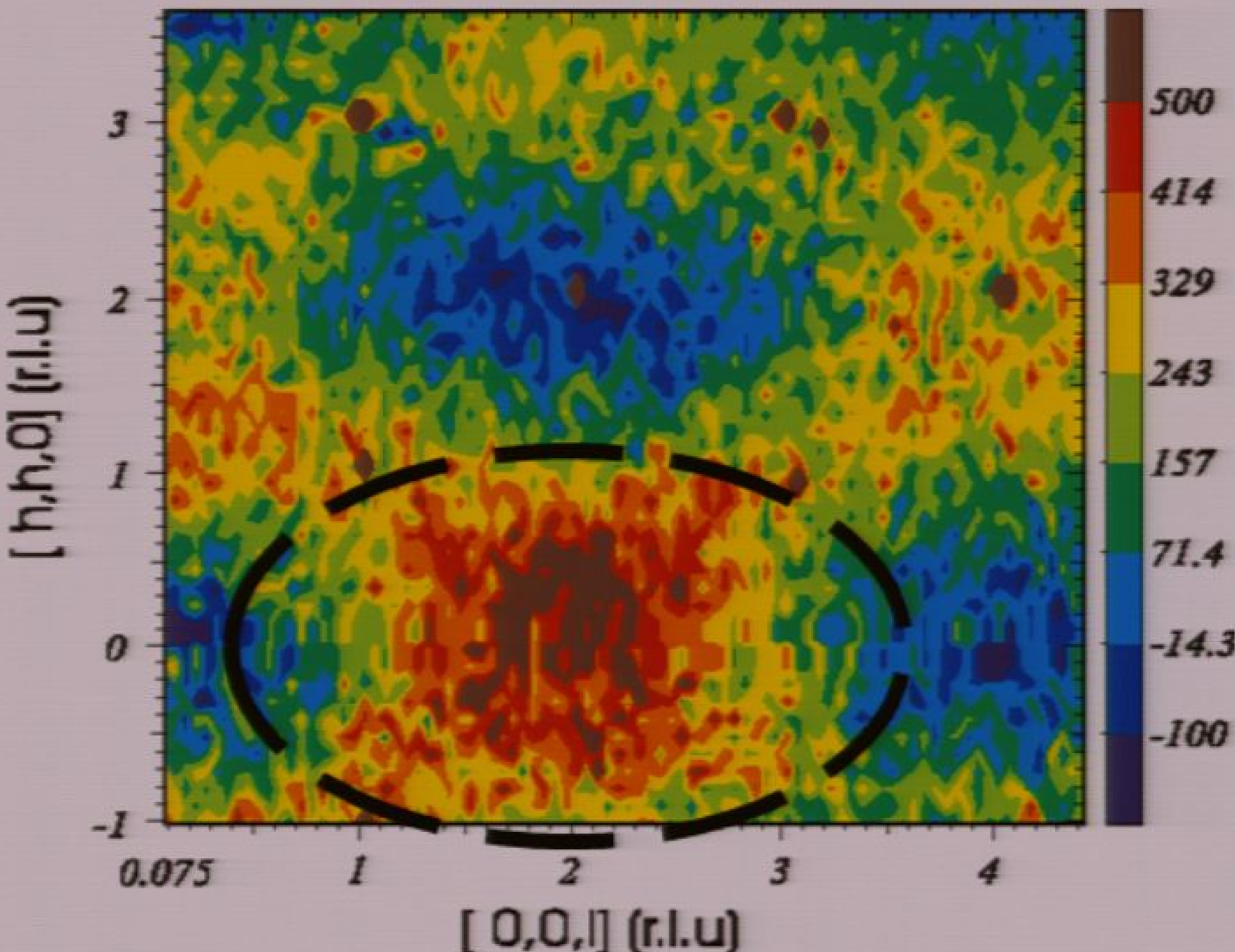


Neutron scattering: no observable sharp magnetic peak appearing from 20 K down to 50 mK (that is a factor 400 in temperature!)



$|m_J\rangle$ wavefunction decomposition

Dy^{3+} (J=15/2) $Dy_2Ti_2O_7$

~350 K

$|\pm 15/2\rangle + O(10^{-1})$

Ho^{3+} (J=8) $Ho_2Ti_2O_7$

~280 K

$|\pm 8\rangle + O(10^{-1})$

$Tb_2Ti_2O_7$

Tb^{3+} (J=6)

$\{ |+3\rangle, |-3\rangle, |+6\rangle, -6\rangle \}$

~20 K

$\{ |+3\rangle, |-3\rangle, |+6\rangle, -6\rangle \}$

~80 K

$|\pm 5\rangle + \varepsilon_e |\pm 2\rangle; \varepsilon_e \sim O(10^{-1})$

~20 K

$|\pm 4\rangle + \varepsilon_g |\pm 1\rangle; \varepsilon_g \sim O(10^{-1})$

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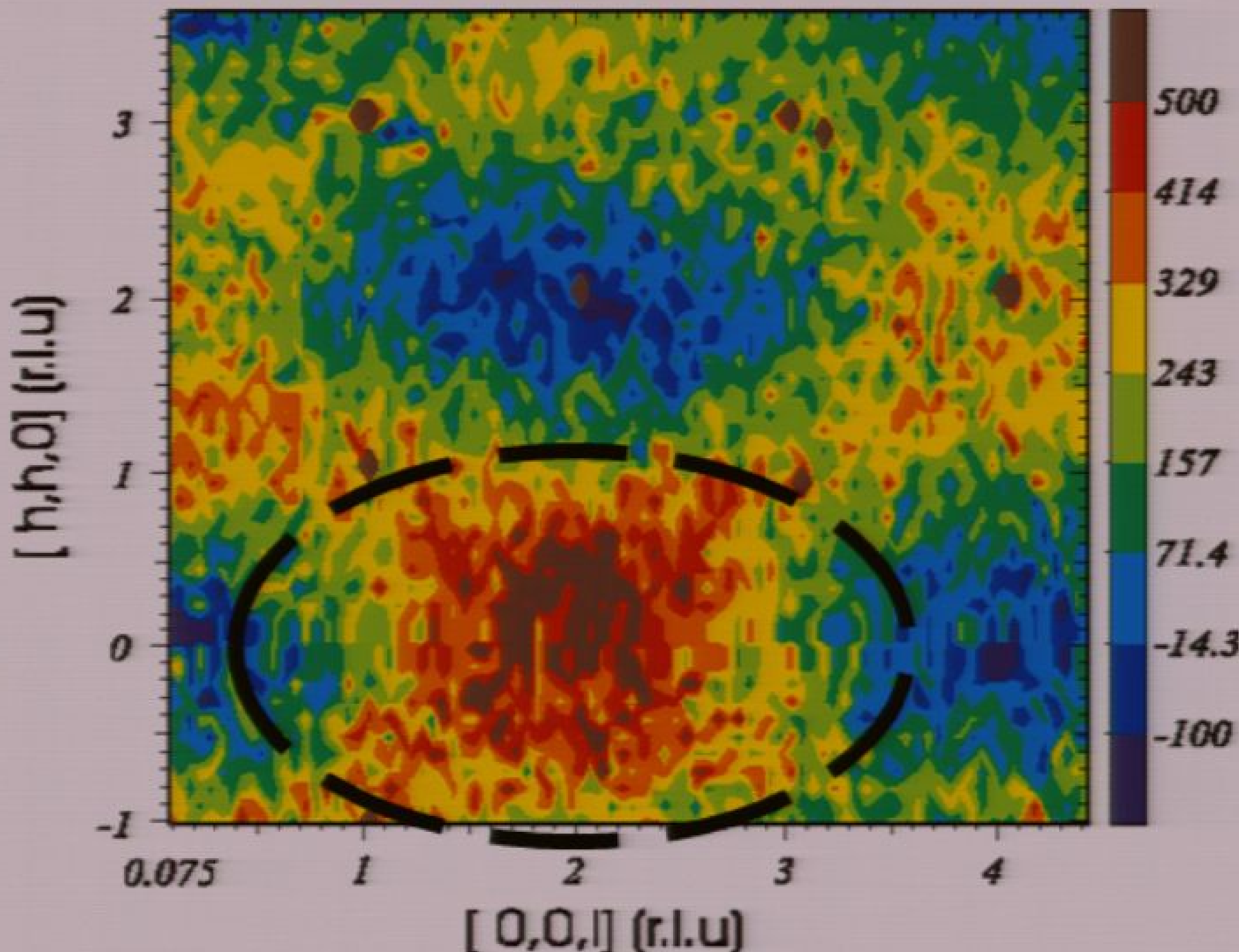

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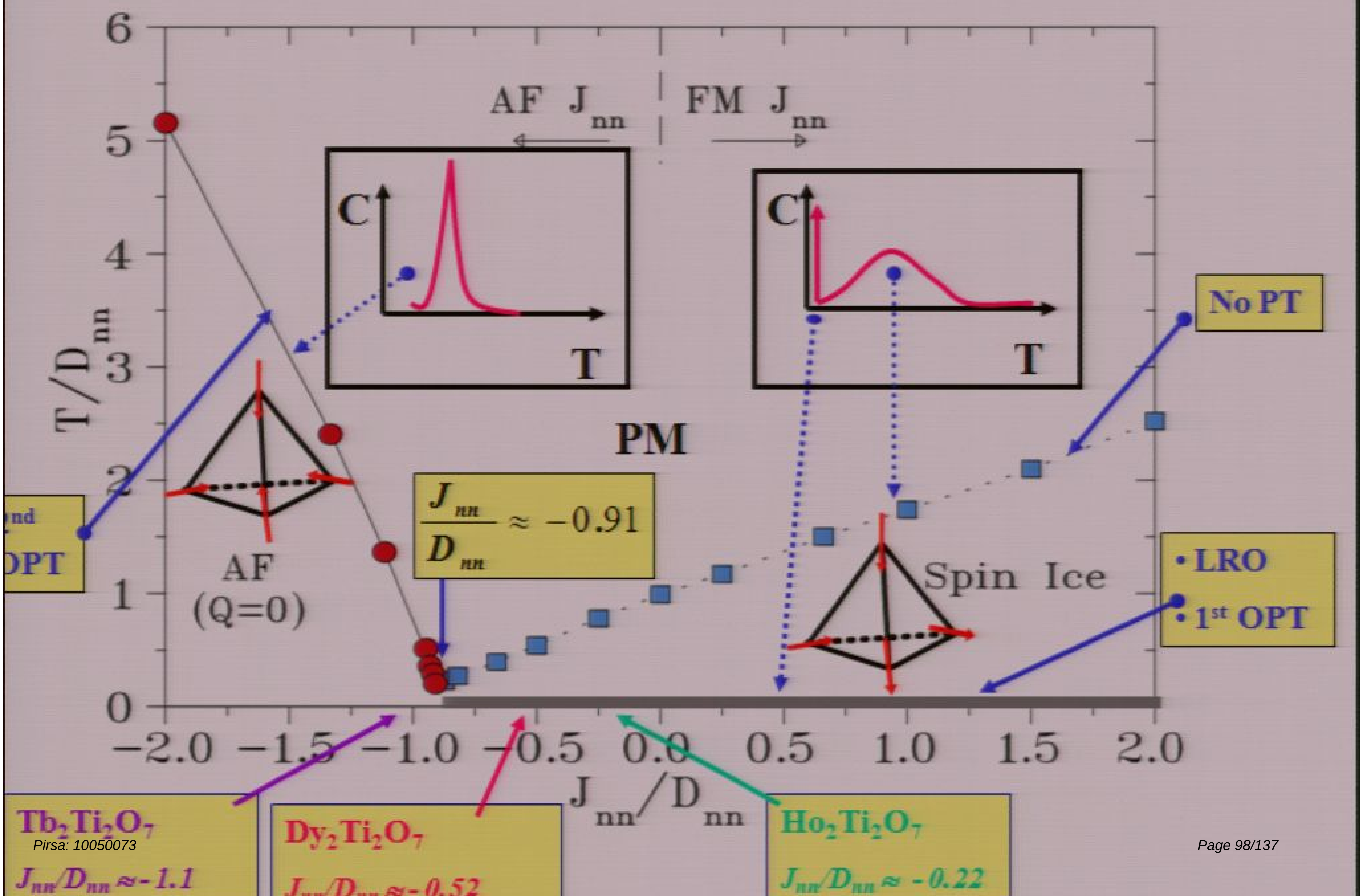

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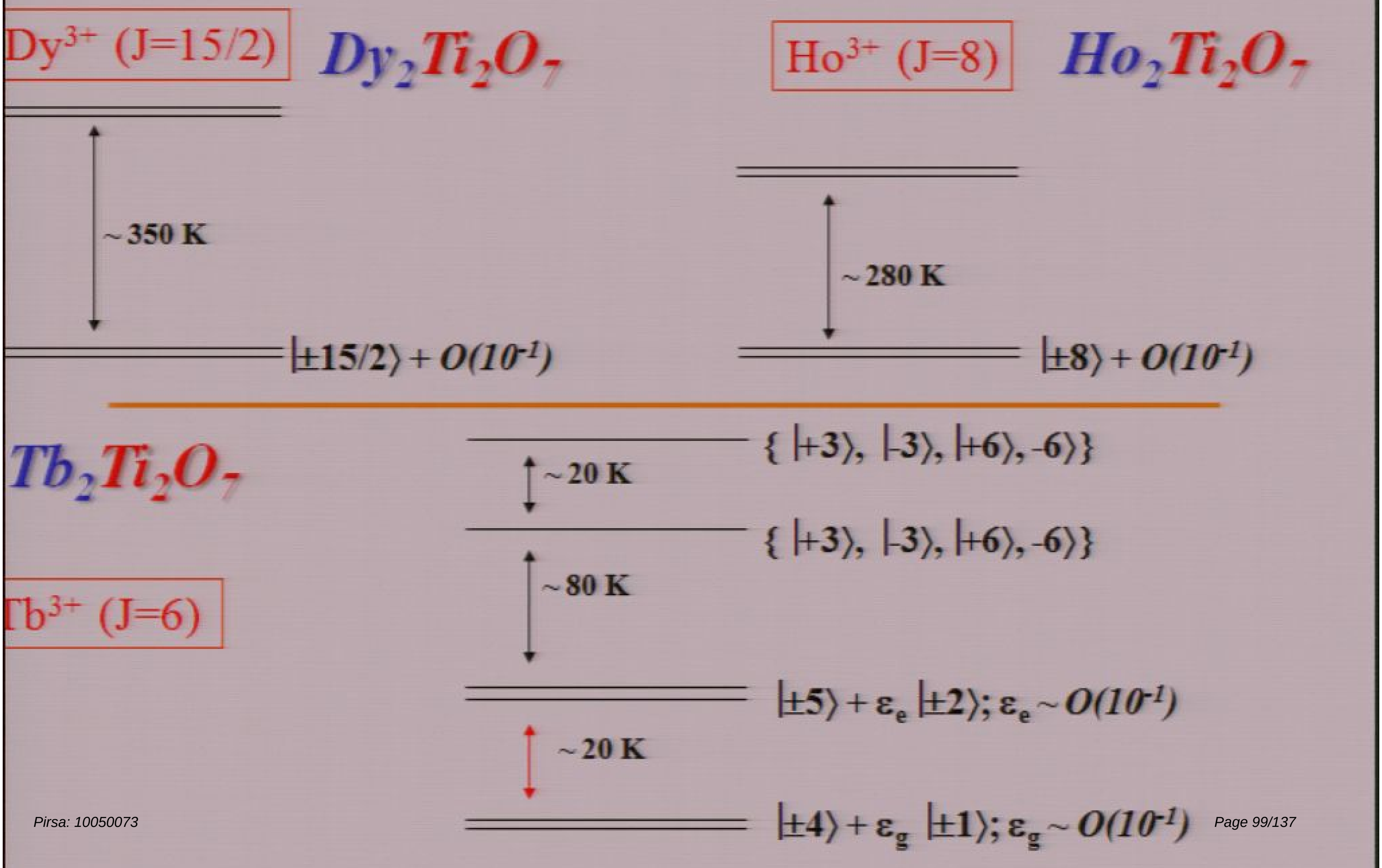

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$|\pm 5\rangle + \varepsilon_e |\pm 2\rangle; \varepsilon_e \sim O(10^{-1})$

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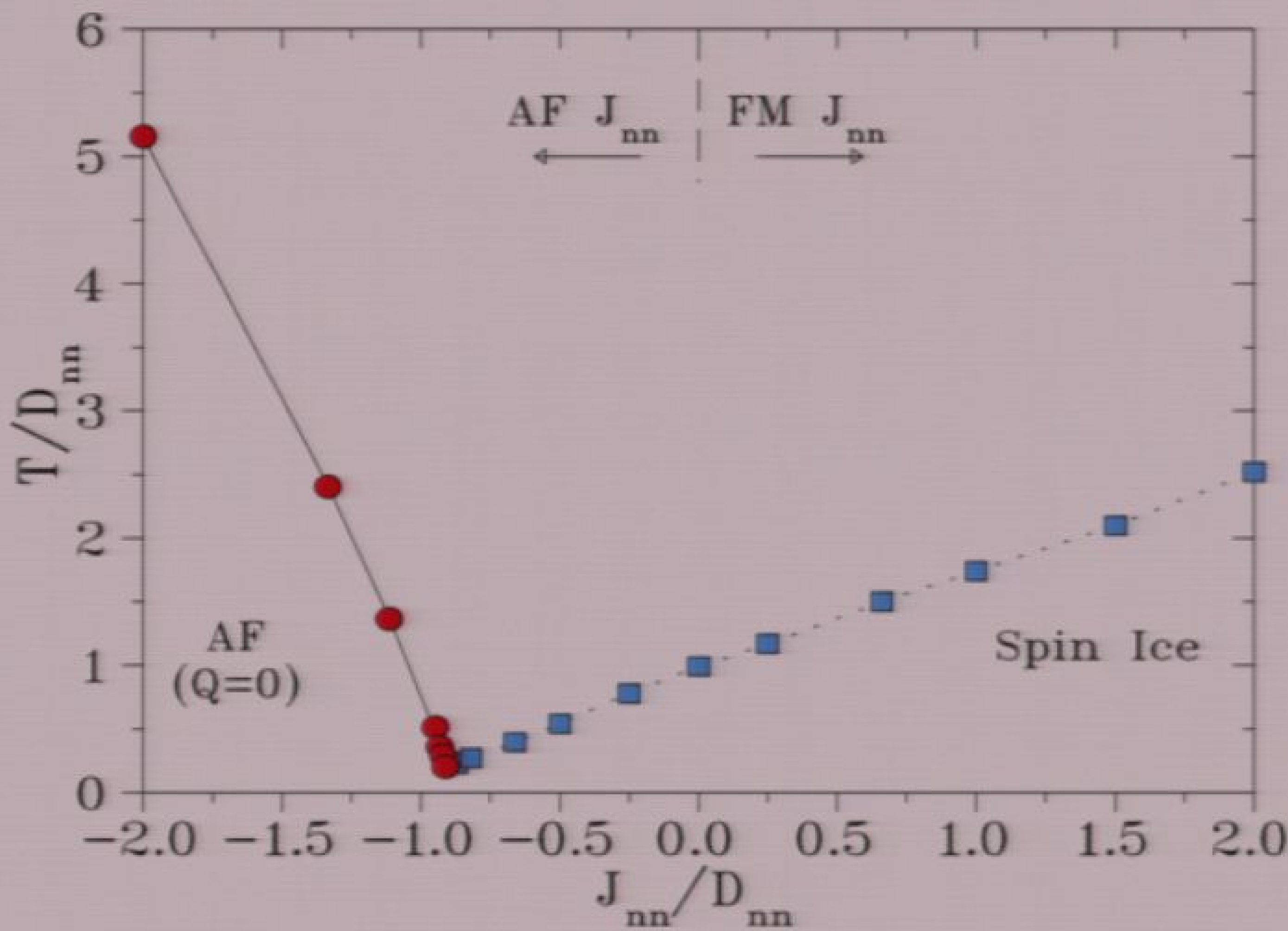
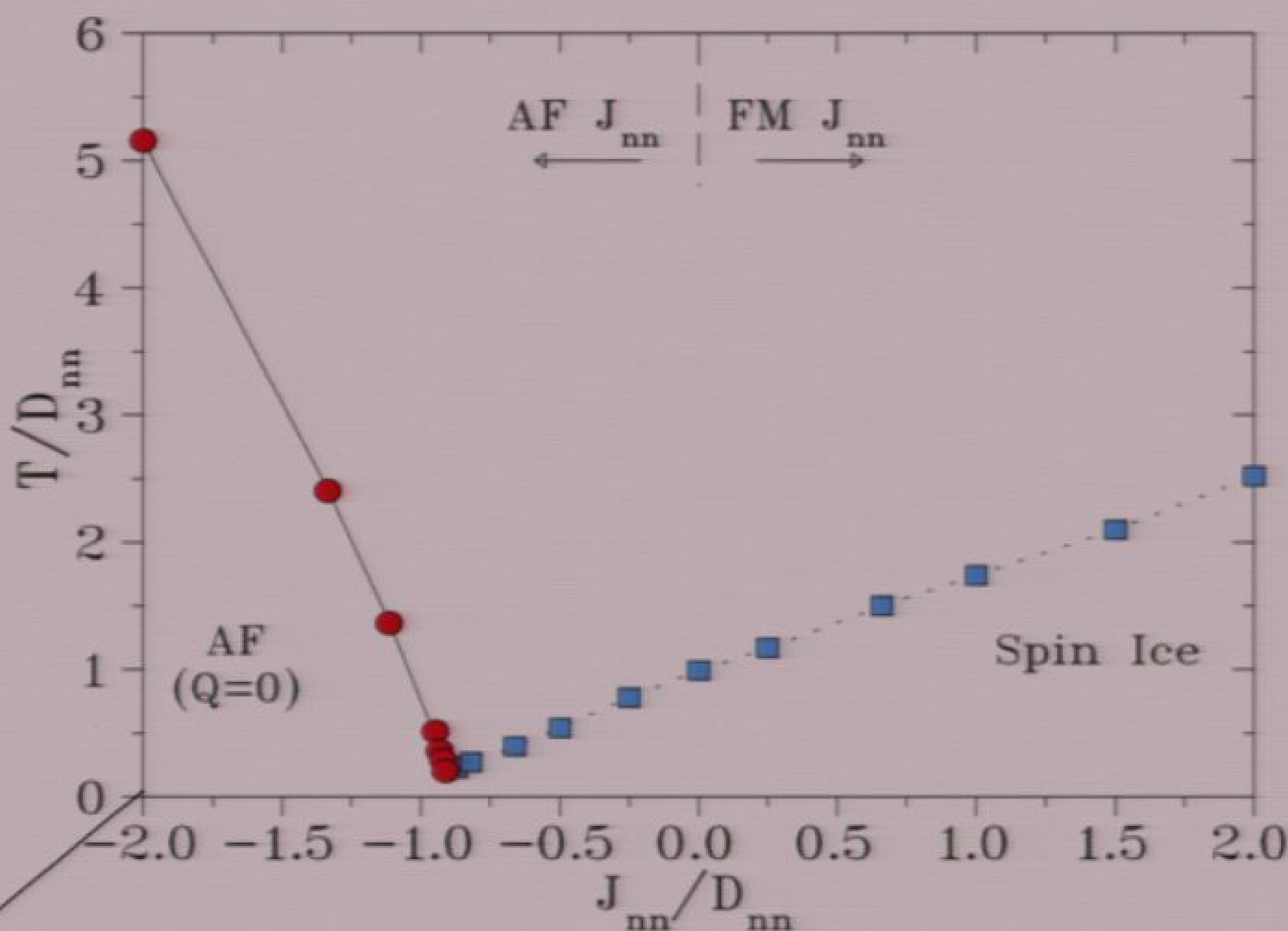
$|\pm 4\rangle + \varepsilon_g |\pm 1\rangle; \varepsilon_g \sim O(10^{-1})$

ingras *et al.*, Phys. Rev. B **61**, 6496 (2000)

Monte Carlo Phase Diagram of the Dipolar Spin Ice Model

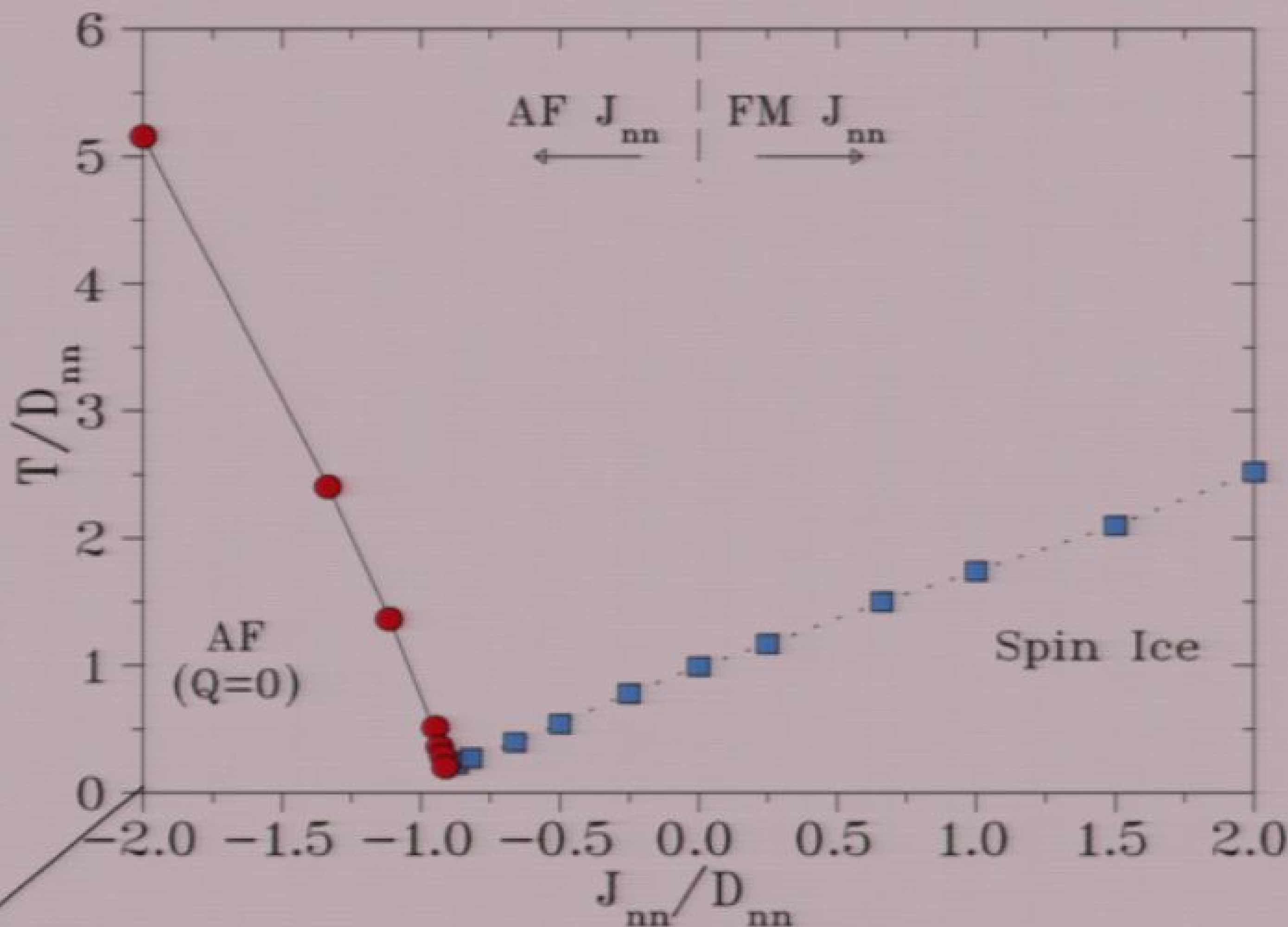


Monte Carlo Phase Diagram of the Dipolar Spin Ice Model



$1/\Delta \sim "\hbar"$

Monte Carlo Phase Diagram of the Dipolar Spin Ice Model



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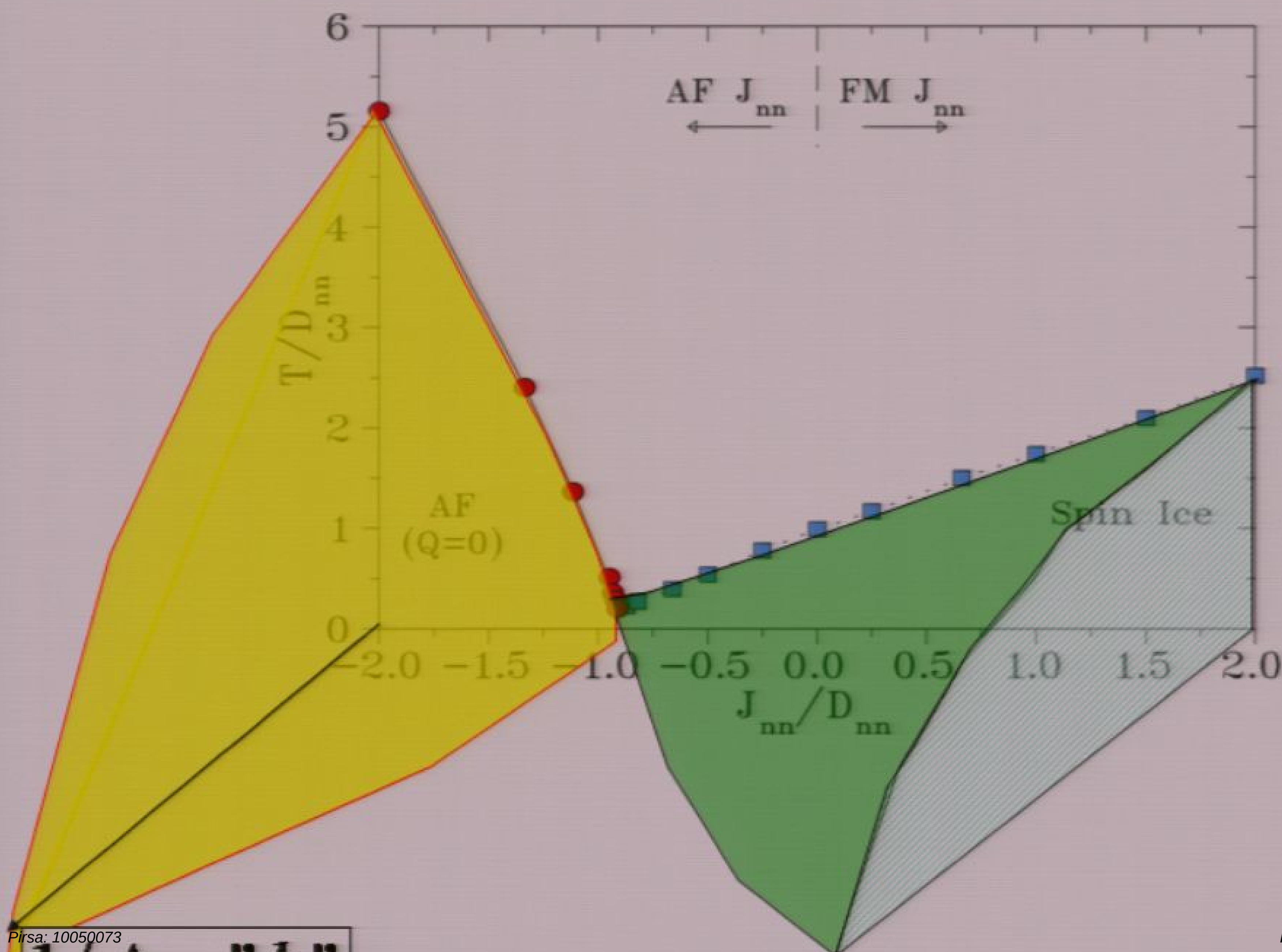
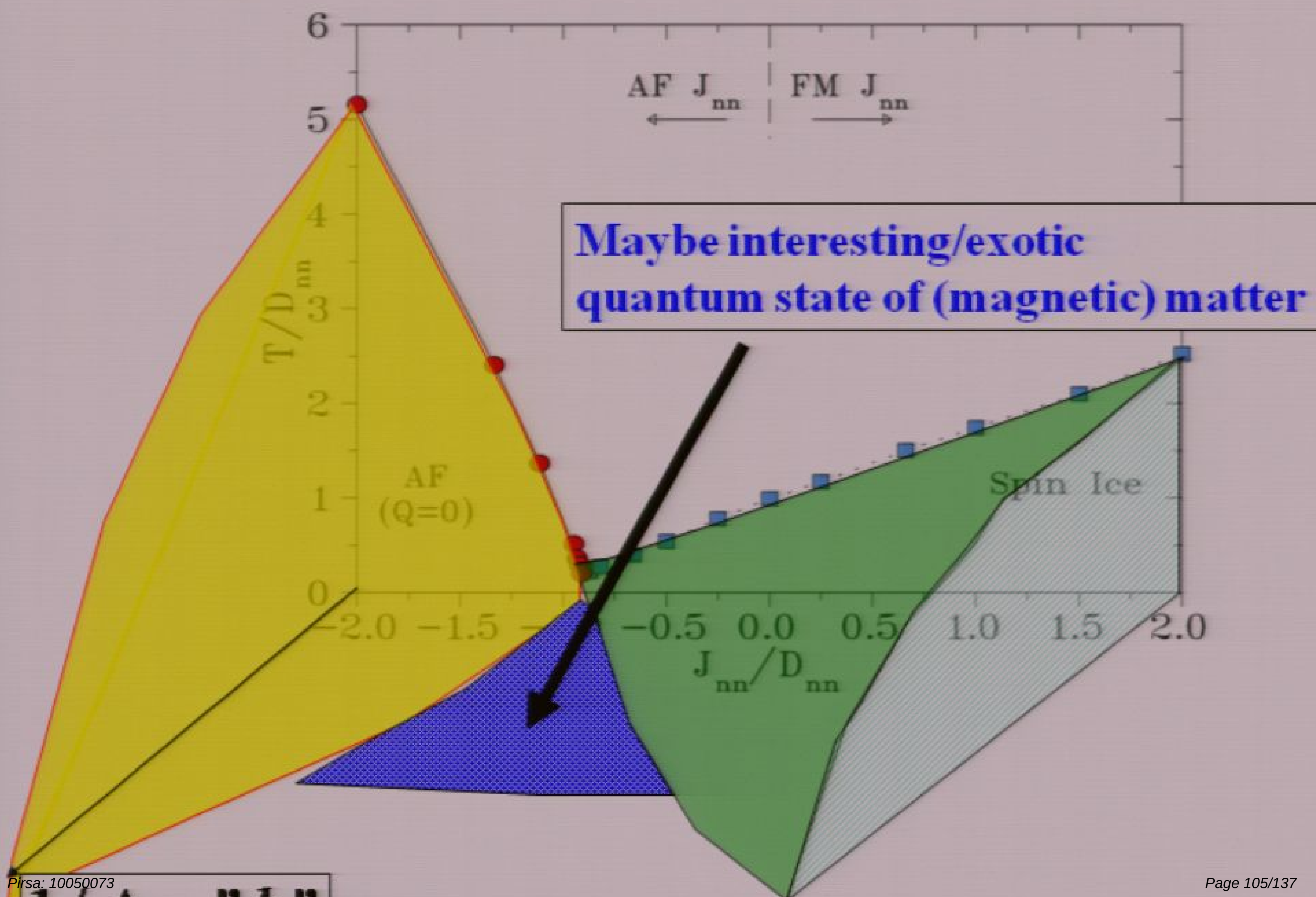


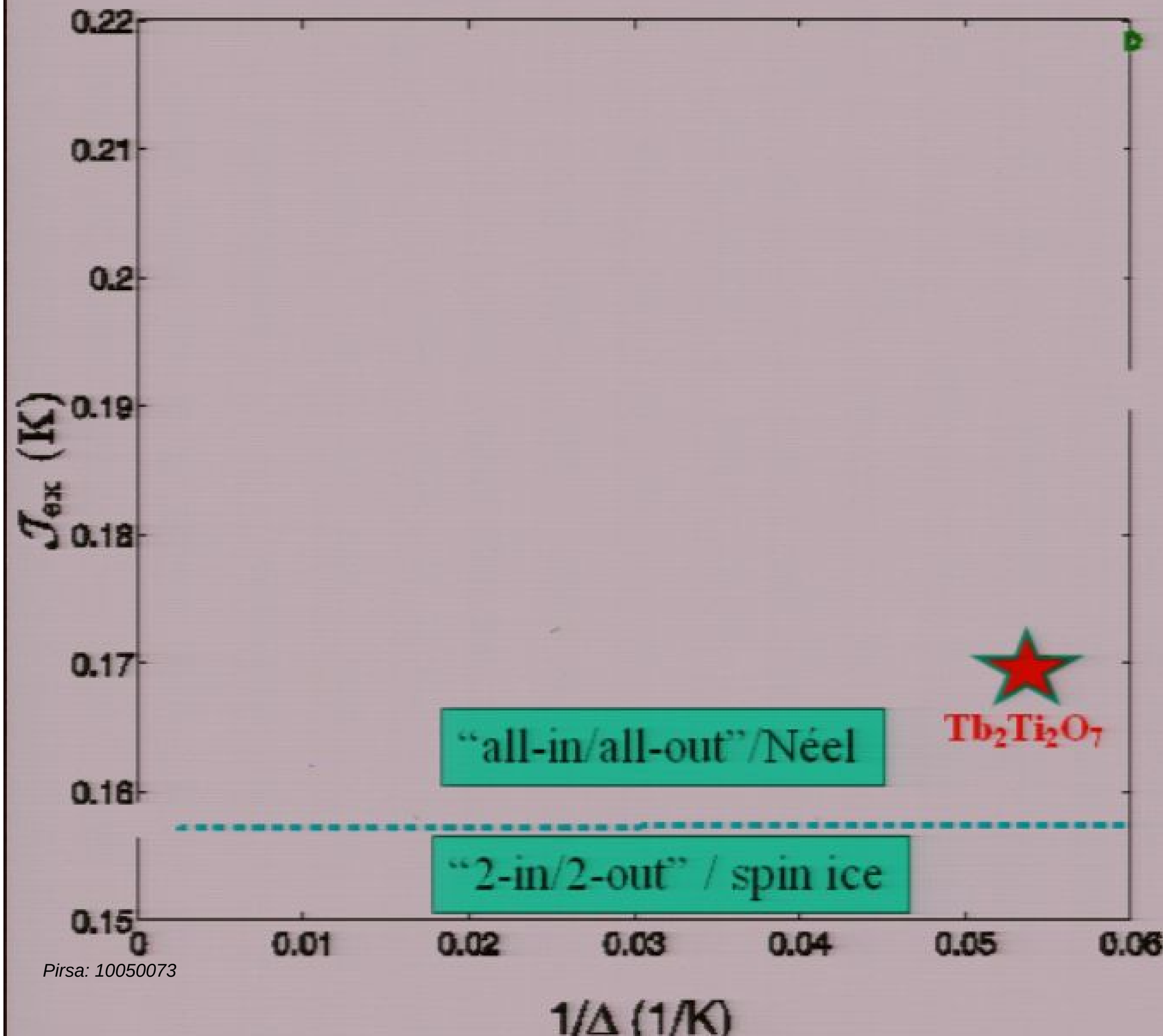
$1/\Delta \sim$ "$\hbar$"

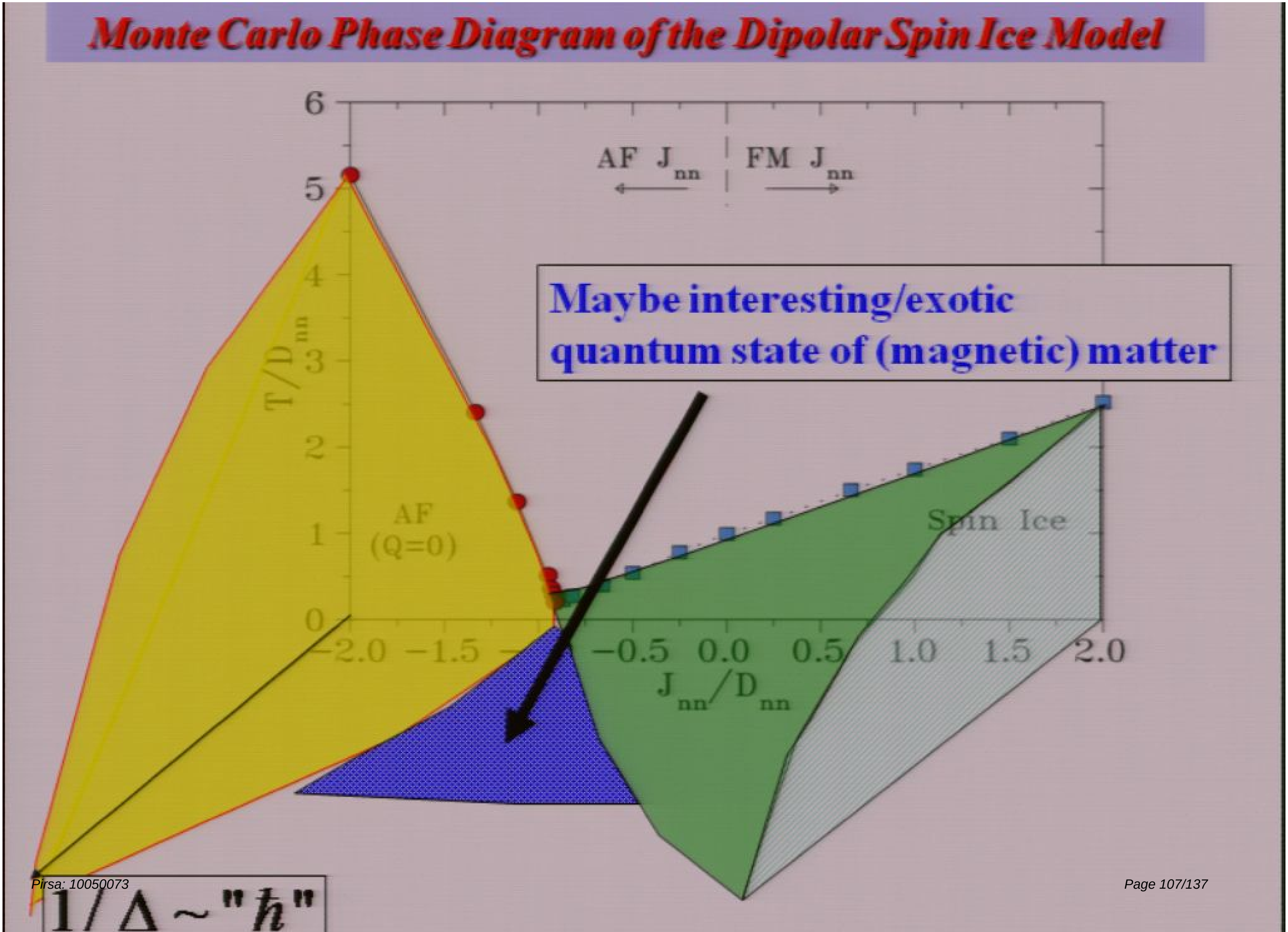
Monte Carlo Phase Diagram of the Dipolar Spin Ice Model



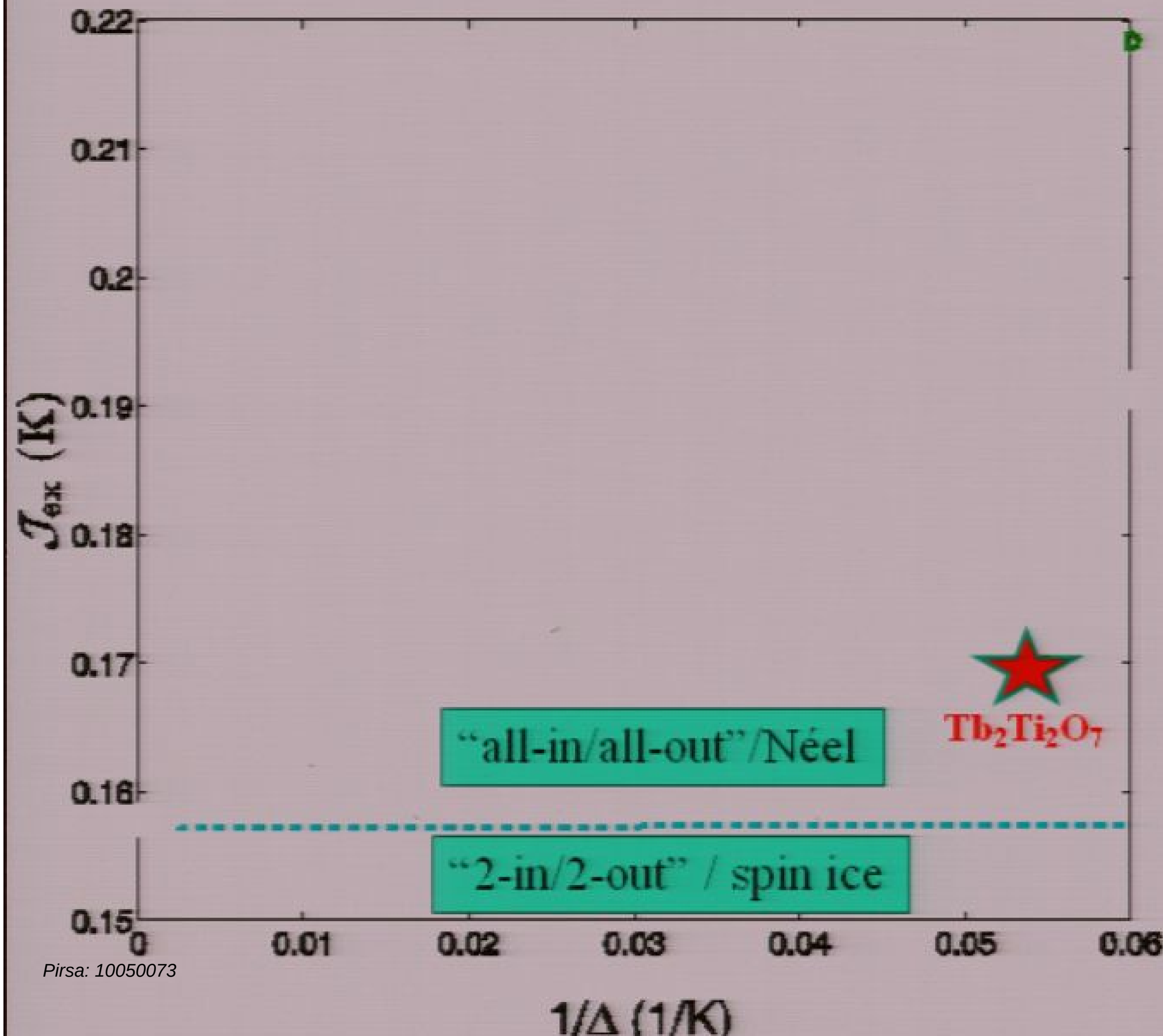
$1/\Delta \sim "\hbar"$

Single tetrahedron phase diagram $Tb_2Ti_2O_7$




Monte Carlo Phase Diagram of the Dipolar Spin Ice Model
Maybe interesting/exotic quantum state of (magnetic) matter
AF J_{nn}
FM J_{nn}
AF (Q=0)
Spin Ice
T/D_{nn}
J_{nn}/D_{nn}
6
5
4
3
2
1
0
−2.0
−1.5
−0.5
0.0
0.5
1.0
1.5
2.0
$1/\Delta \sim "\hbar"$

Single tetrahedron phase diagram $Tb_2Ti_2O_7$



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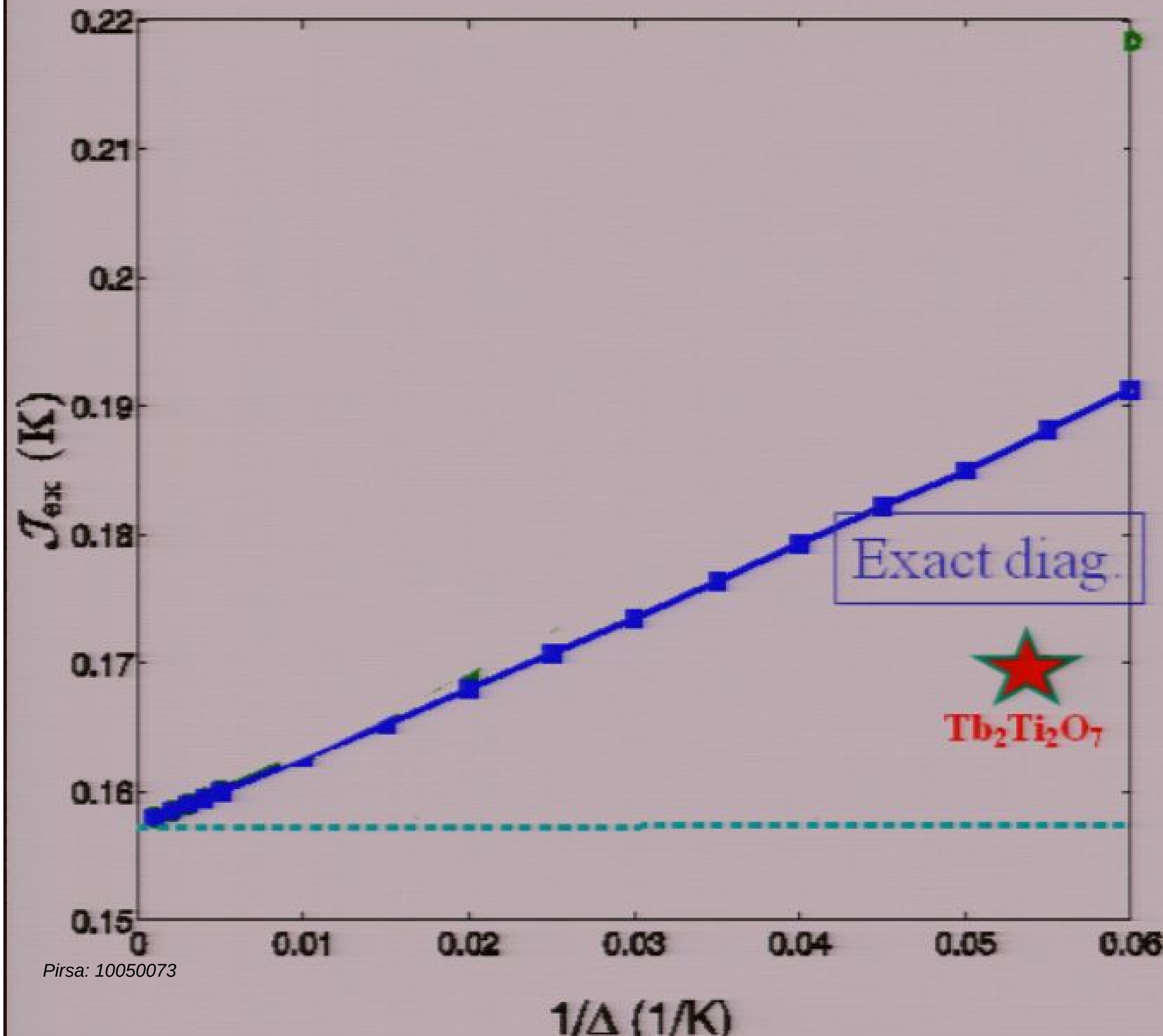

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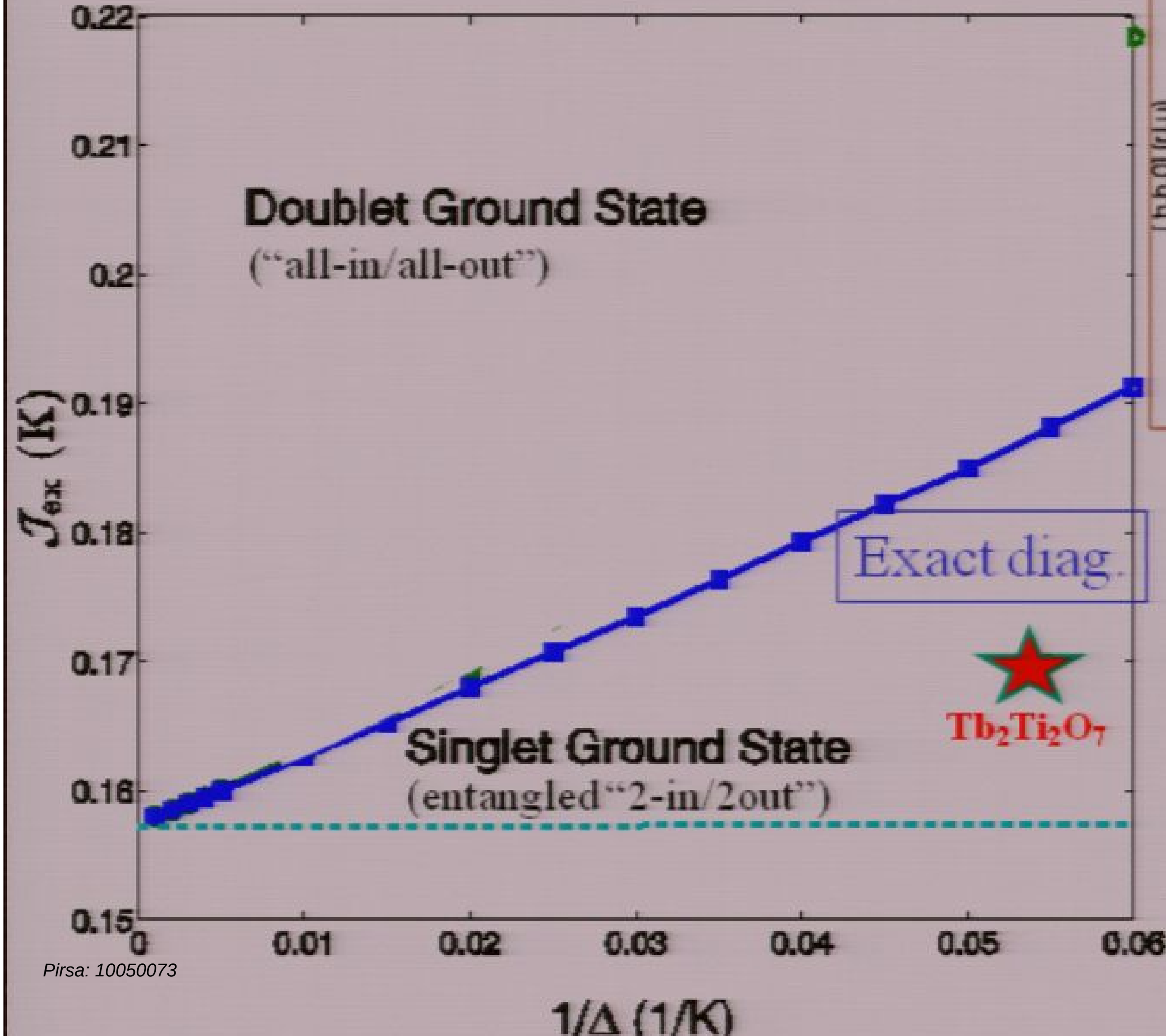
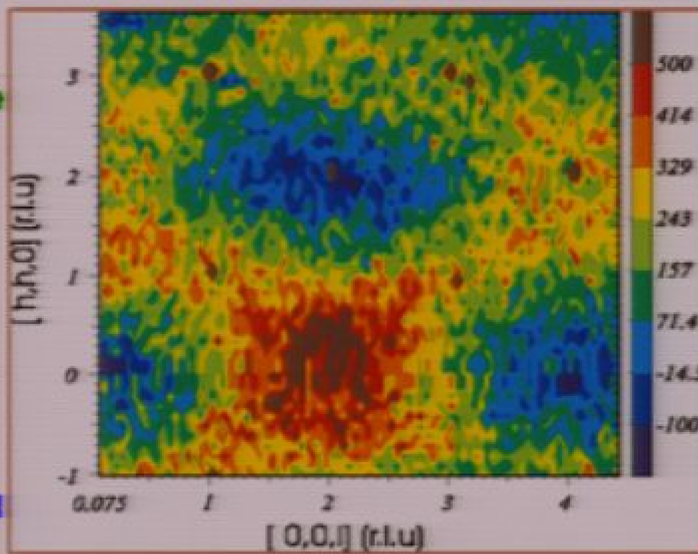




Elimination of high energy sector

$$H = H_{\mathrm{cf}} + V,\ V \ll H_{\mathrm{cf}}$$

Effective Hamiltonian Method

$$V = J_{ex} \sum_{\langle i,j \rangle} \vec{J}_i \bullet \vec{J}_j + D R_{nn}^3 \sum_{\substack{i,j \\ j>i}} \left\{ \frac{(\vec{J}_i \bullet \vec{J}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{J}_i \bullet \vec{R}_{ij})(\vec{R}_{ij} \bullet \vec{J}_j)}{|\vec{R}_{ij}|^5} \right\}$$

H_{ex} H_{dip}

Effective Hamiltonian Method

$$V = J_{ex}\sum_{\langle i,j\rangle}\vec{J}_i\bullet\vec{J}_j + DR_{nn}^3\sum_{\substack{i,j\\ j>i}}\left\{\frac{(\vec{J}_i\bullet\vec{J}_j)}{|\vec{R}_{ij}|^3}-\frac{3(\vec{J}_i\bullet\vec{R}_{ij})(\vec{R}_{ij}\bullet\vec{J}_j)}{|\vec{R}_{ij}|^5}\right\}$$

H_{ex} $\quad$ H_{dip}

$$H_{\mathrm{eff}} = PVP + PVQVP + \cdots$$

$$\mathbf{P} = \sum_{\alpha\in\mathbf{P}}|\alpha\rangle\langle\alpha|$$

$$Q = \sum_{\beta\notin P}\frac{|\beta\rangle\langle\beta|}{E_0^{\alpha}-E_0^{\beta}}$$

$$H_{\mathrm{eff}} = PH_{\mathrm{ex}}P + PH_{\mathrm{dip}}P + PH_{\mathrm{ex}}QH_{\mathrm{ex}}P$$
$$+(PH_{\mathrm{ex}}QH_{\mathrm{dip}}P + PH_{\mathrm{dip}}QH_{\mathrm{ex}}P) + PH_{\mathrm{dip}}QH_{\mathrm{dip}}P$$

Effective Hamiltonian Method

$$V = J_{ex}\sum_{\langle i,j\rangle} \vec{J}_i \bullet \vec{J}_j + DR_{nn}^3 \sum_{\substack{i,j\\ j>i}} \left\{ \frac{(\vec{J}_i \bullet \vec{J}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{J}_i \bullet \vec{R}_{ij})(\vec{R}_{ij} \bullet \vec{J}_j)}{|\vec{R}_{ij}|^5} \right\}$$

H_{ex} H_{dip}

$$H_{eff} = PVP + PVQVP + \cdots$$

$$\mathbf{P} = \sum_{\alpha\in \mathbf{P}} |\alpha\rangle\langle\alpha|$$

Large denominator compared to the energy scale of H'

$$Q = \sum_{\beta\notin P} \frac{|\beta\rangle\langle\beta|}{E_0^{\alpha} - E_0^{\beta}}$$

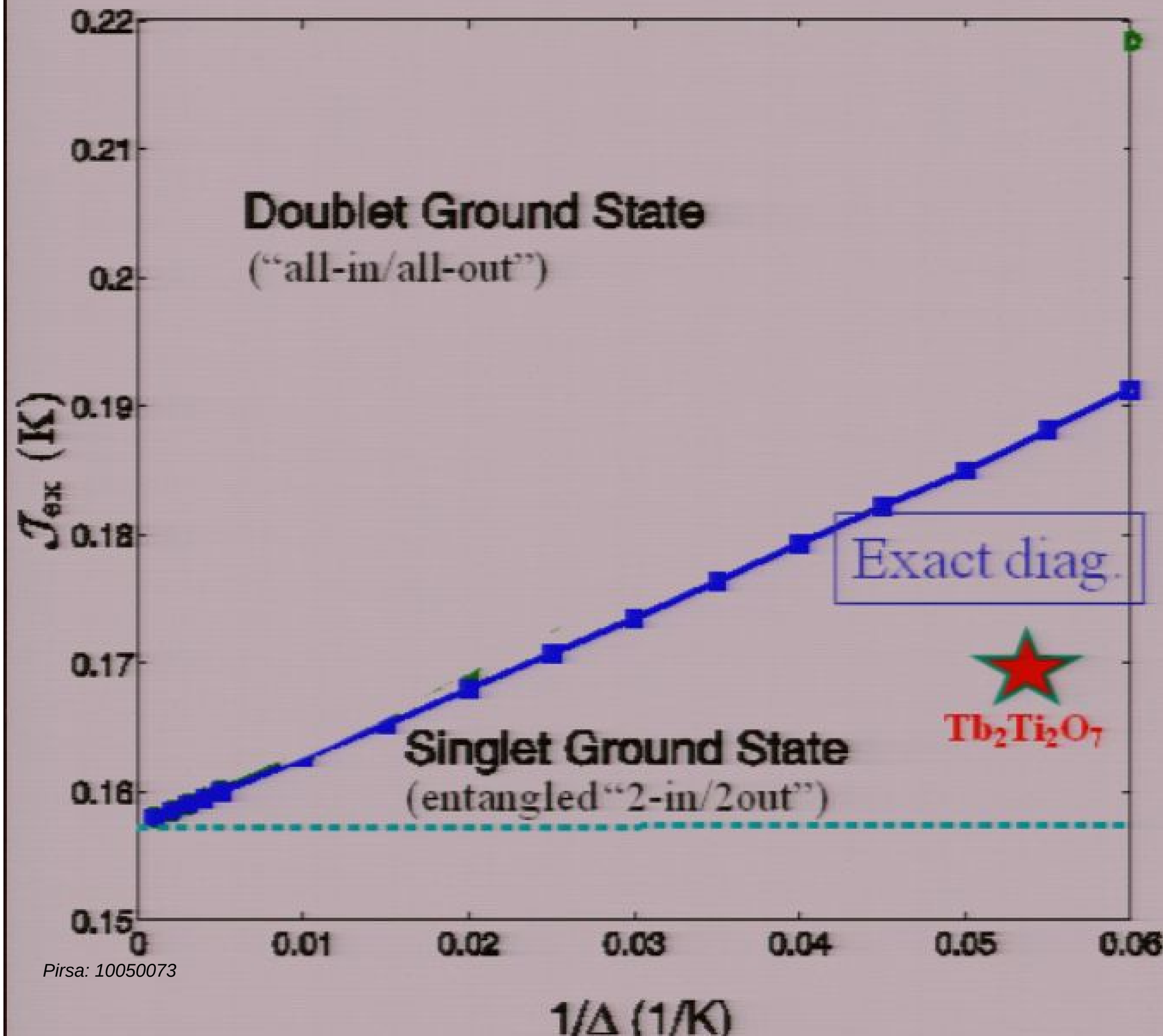
$$H_{eff} = PH_{ex}P + PH_{dip}P + PH_{ex}QH_{ex}P$$
$$+(PH_{ex}QH_{dip}P + PH_{dip}QH_{ex}P) + PH_{dip}QH_{dip}P$$

Effective spin-1/2 (XXZ) model

$$H_{\text{eff}} = \sum_{i>j} J_{ij}^{z_i z_j}\left(r_{ij}\right) S_i^{z_i} S_j^{z_j} + \sum_{\substack{i>j \\ u\neq v\neq z}} J_{ij}^{u_i v_j}\left(r_{ij}\right) S_i^{u_i} S_j^{v_j}$$

pseudo spin-1/2 model

Single tetrahedron phase diagram $Tb_2Ti_2O_7$



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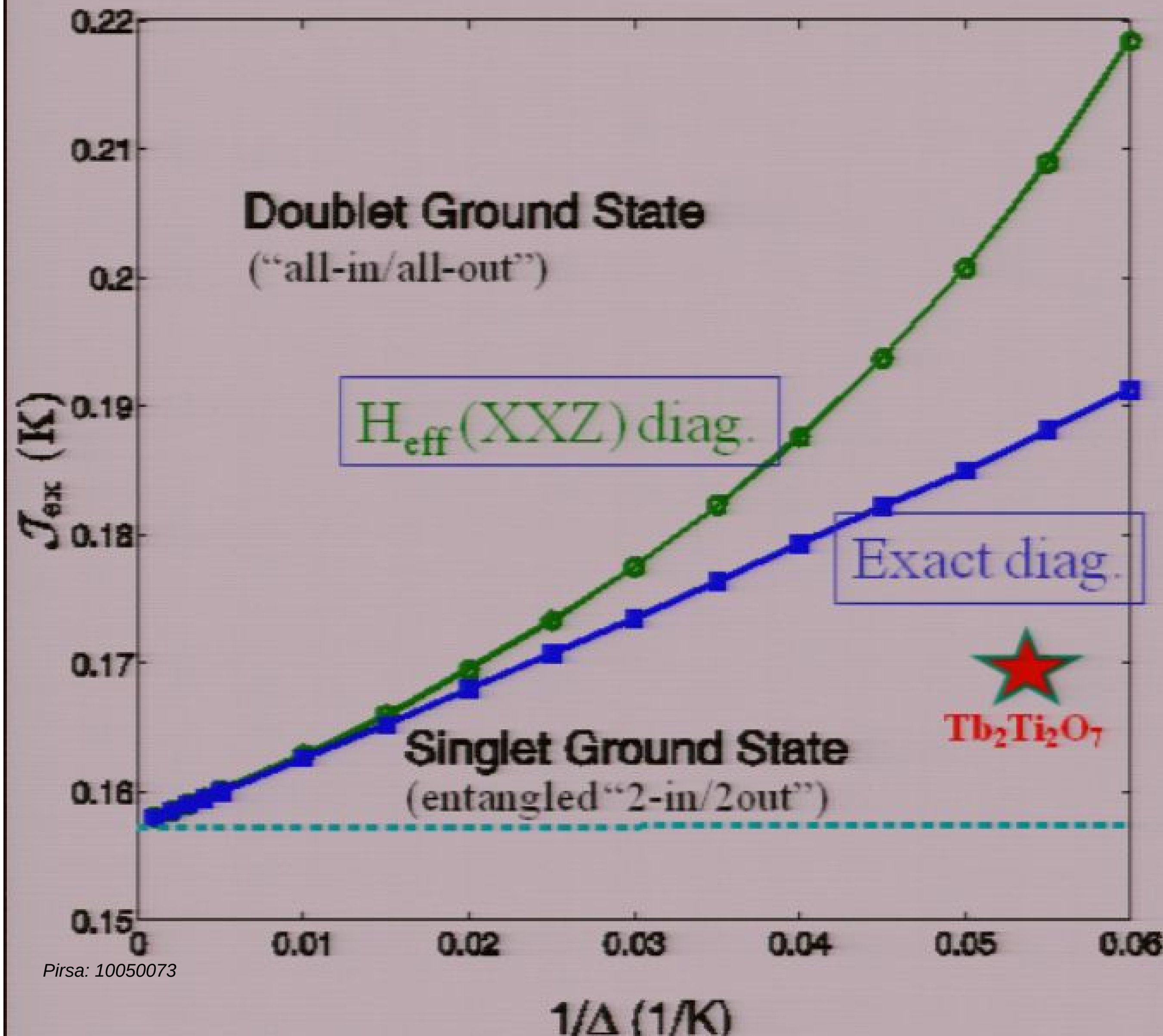

Effective spin-1/2 (XXZ) model

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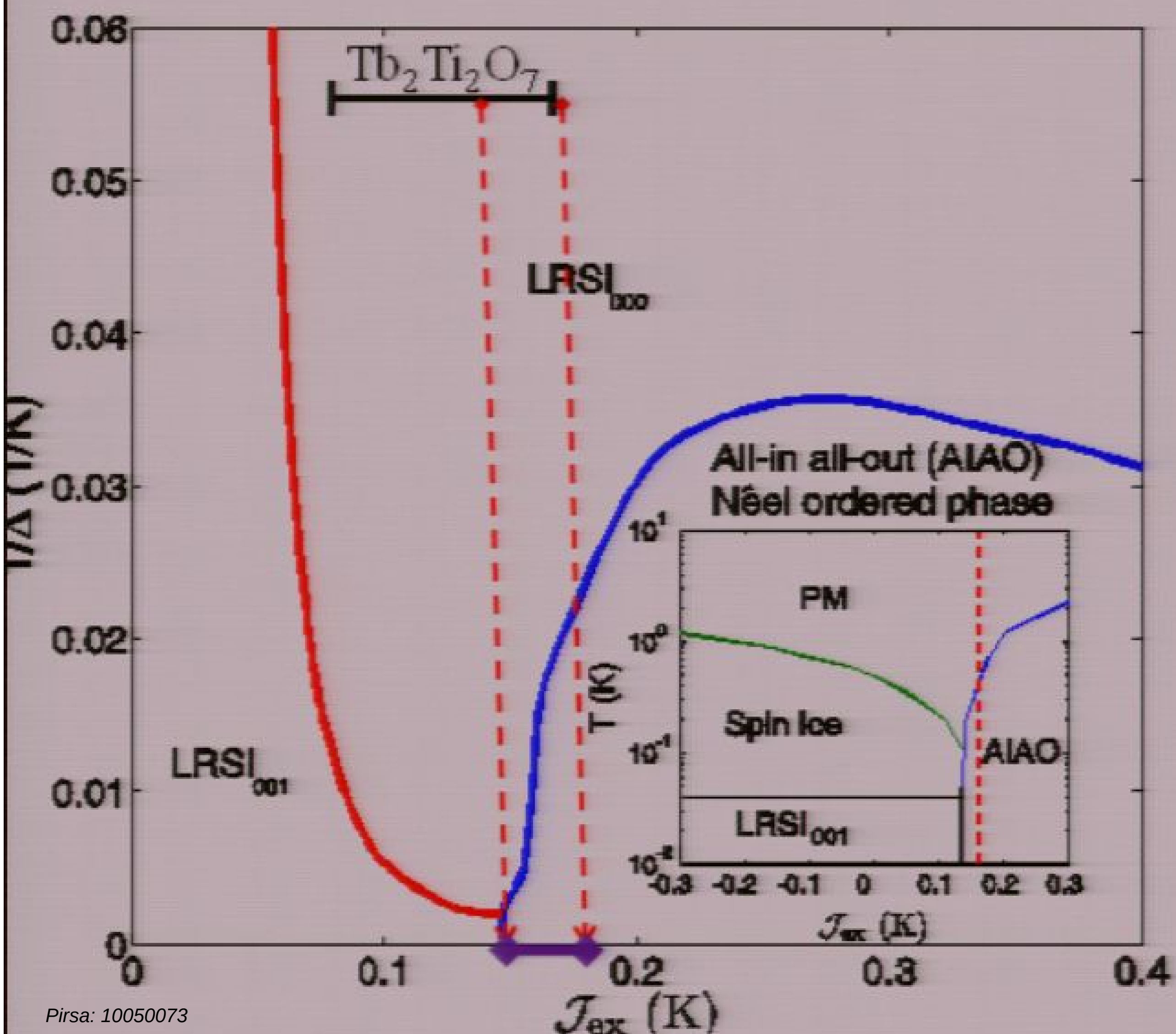
$$H_{\rm eff} = \sum_{i>j} J_{ij}^{z_i z_j}\left(r_{ij}\right) S_i^{z_i} S_j^{z_j} + \sum_{\substack{i>j\\ u\neq v\neq z}} J_{ij}^{u_i v_j}\left(r_{ij}\right) S_i^{u_i} S_j^{v_j}$$

pseudo spin-1/2 model

<u>But now, on the lattice, not only on a single tetrahedron</u>

Semi-classical phase diagram of $Tb_2Ti_2O_7$ on the lattice



Simpler phenomenological model – not derived

$$H' = H_{\text{ex}} + H_{\text{dip}}$$

$$H_{\text{ex}} = J_{\text{ex}} \sum_{\langle i,j \rangle} \vec{J}_i \bullet \vec{J}_j$$

$$H_{\text{dip}} = D R_{nn}^3 \sum_{\substack{i,j \\ j>i}} \left\{ \frac{(\vec{J}_i \bullet \vec{J}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{J}_i \bullet \vec{R}_{ij})(\vec{R}_{ij} \bullet \vec{J}_j)}{|\vec{R}_{ij}|^5} \right\}$$

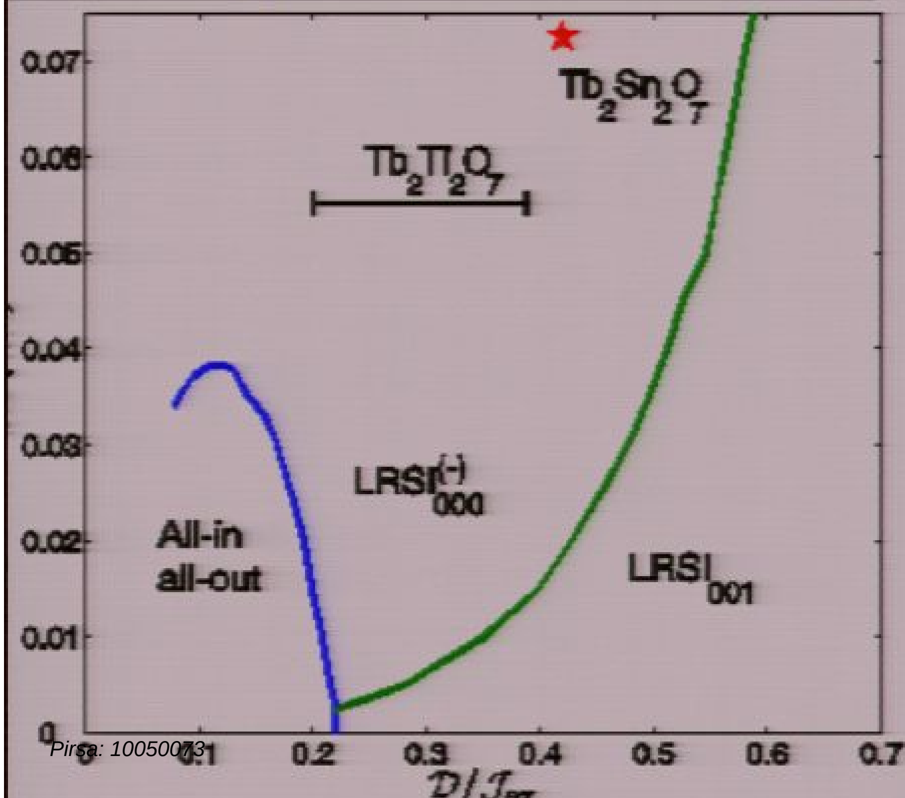
$$\vec{J}_i = \left(\eta S_i^{x_i}, \eta S_i^{y_i}, (1-\eta) S_i^{z_i} \right)$$

- η=0 : Ising limit
- η=1/2: Heisenberg limit
- η=1 : XY limit

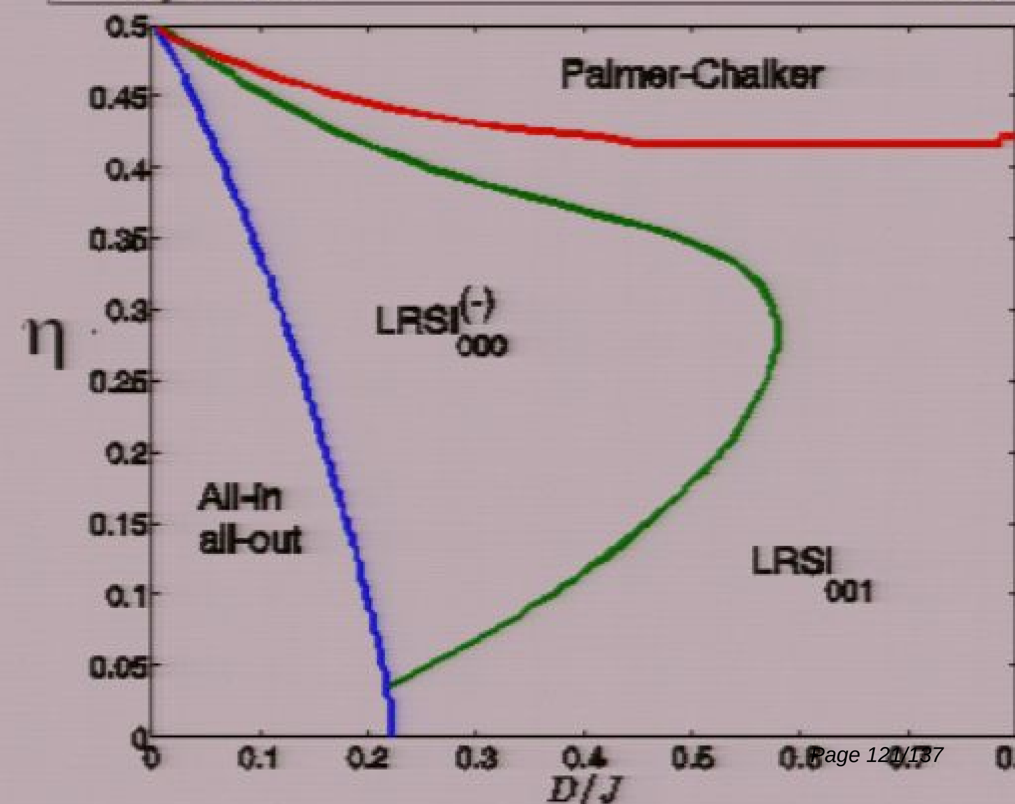
Simpler phenomenological model – not derived

$$H' = J_{ex} \sum_{\langle i,j \rangle} \vec{J}_i \bullet \vec{J}_j + D R_{nn}^3 \sum_{\substack{i,j \\ j>i}} \left\{ \frac{(\vec{J}_i \bullet \vec{J}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{J}_i \bullet \vec{R}_{ij})(\vec{R}_{ij} \bullet \vec{J}_j)}{|\vec{R}_{ij}|^5} \right\}$$

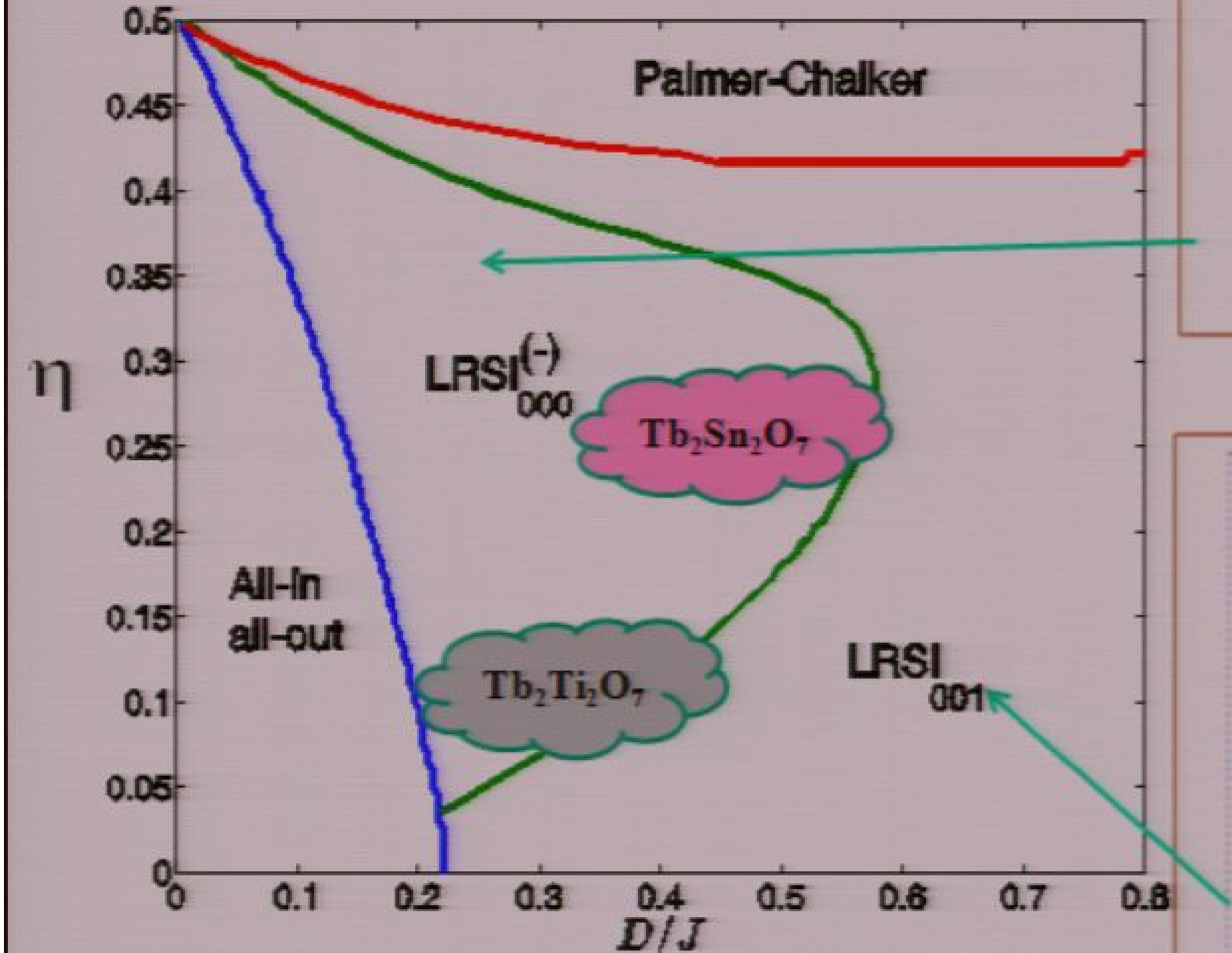
From H_{eff} derived from H_{micro}

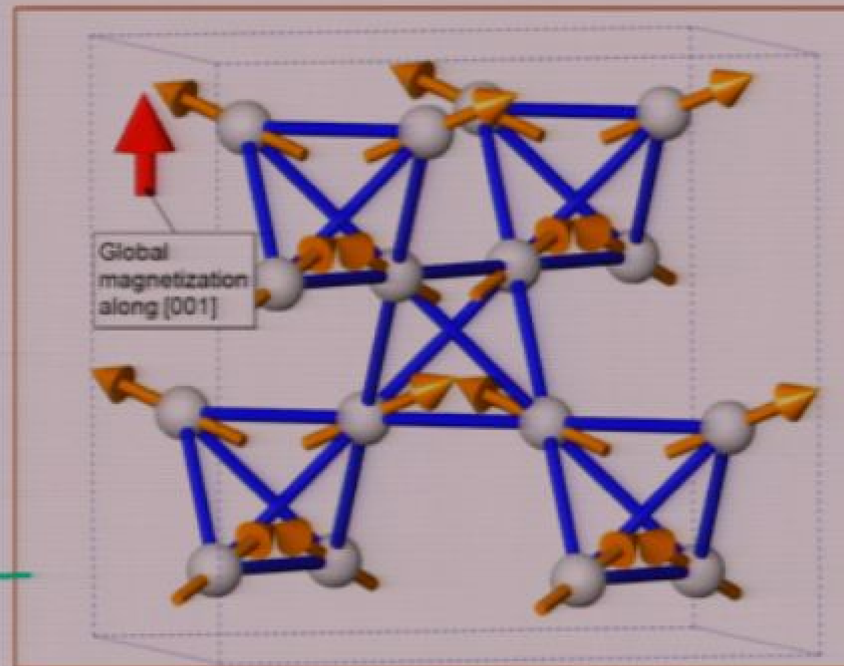


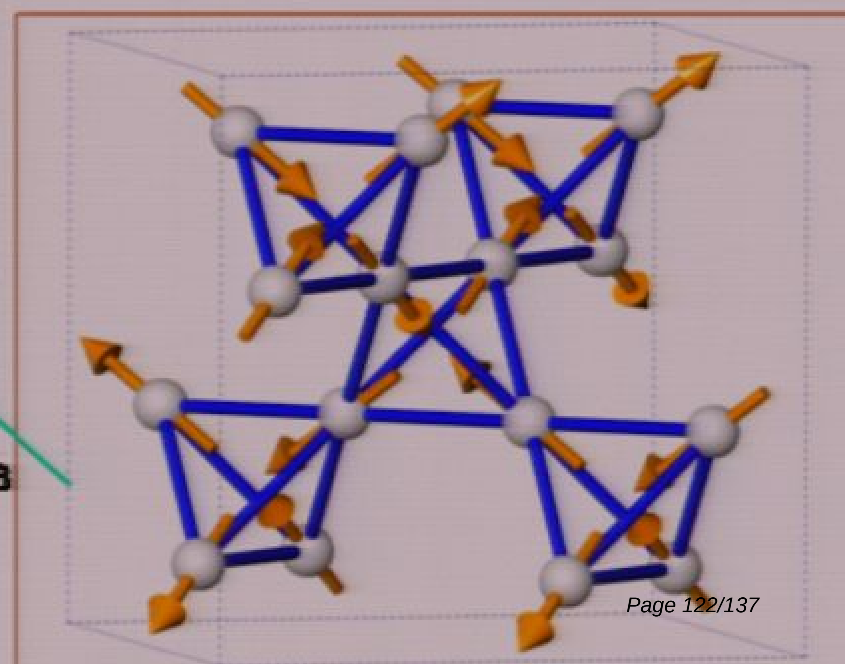
$H_{\text{toy-model}}$ <u>not</u> derived from H_{micro}



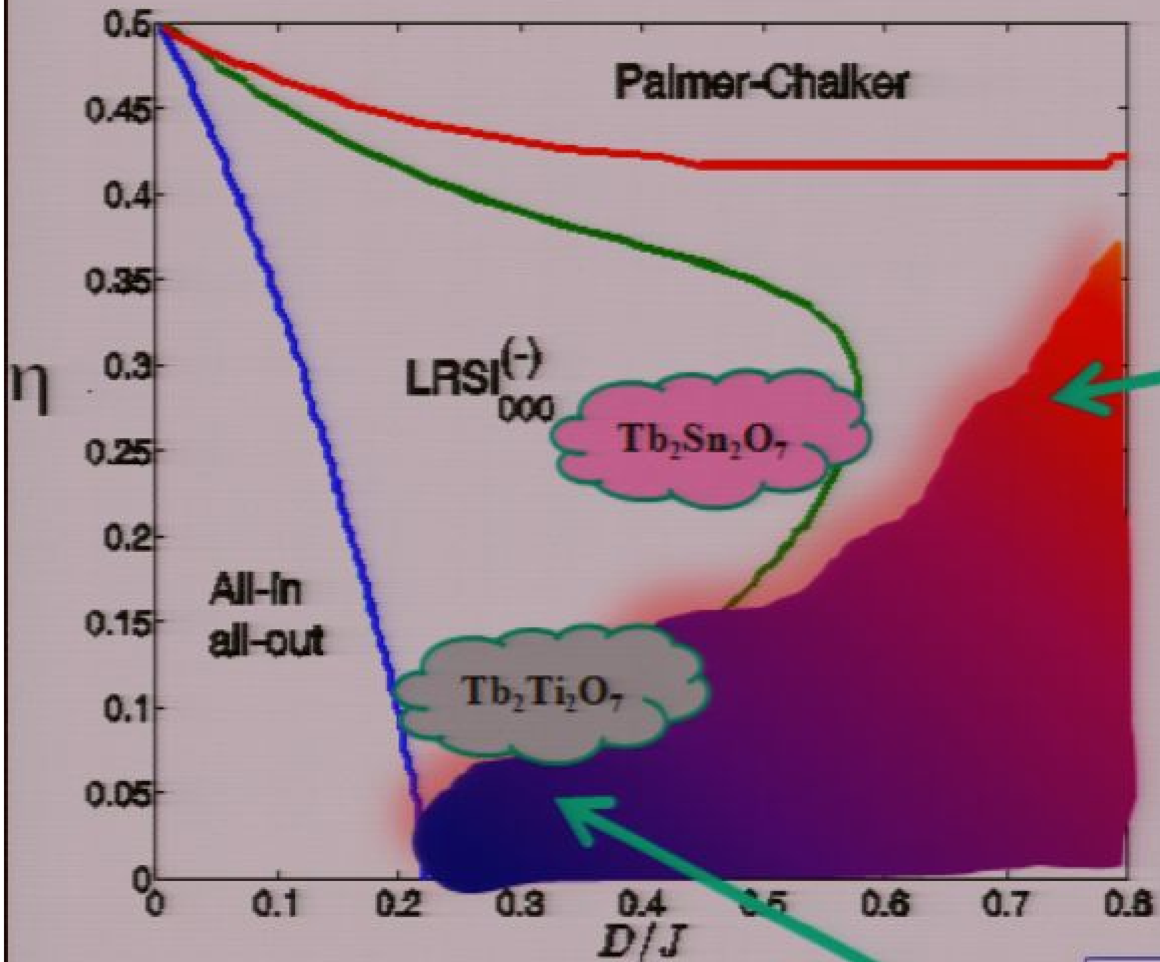
Simpler phenomenological model







Simpler phenomenological model



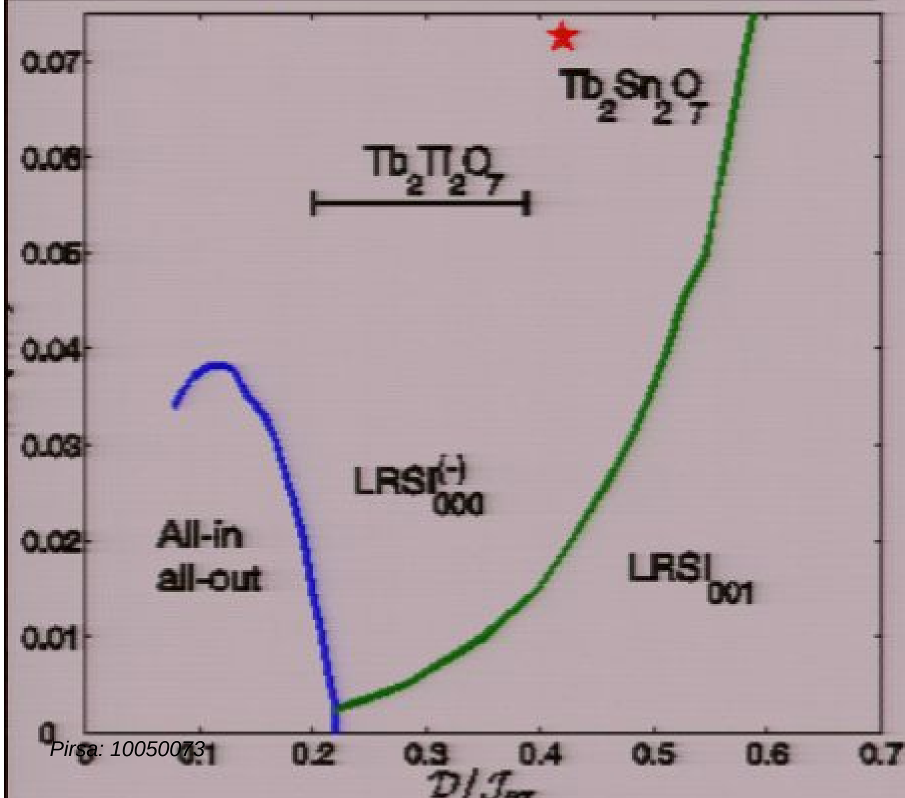
Can hardly reach
that state when cooling
from paramagnetic phase

Cannot reach that state when cooling
from paramagnetic phase

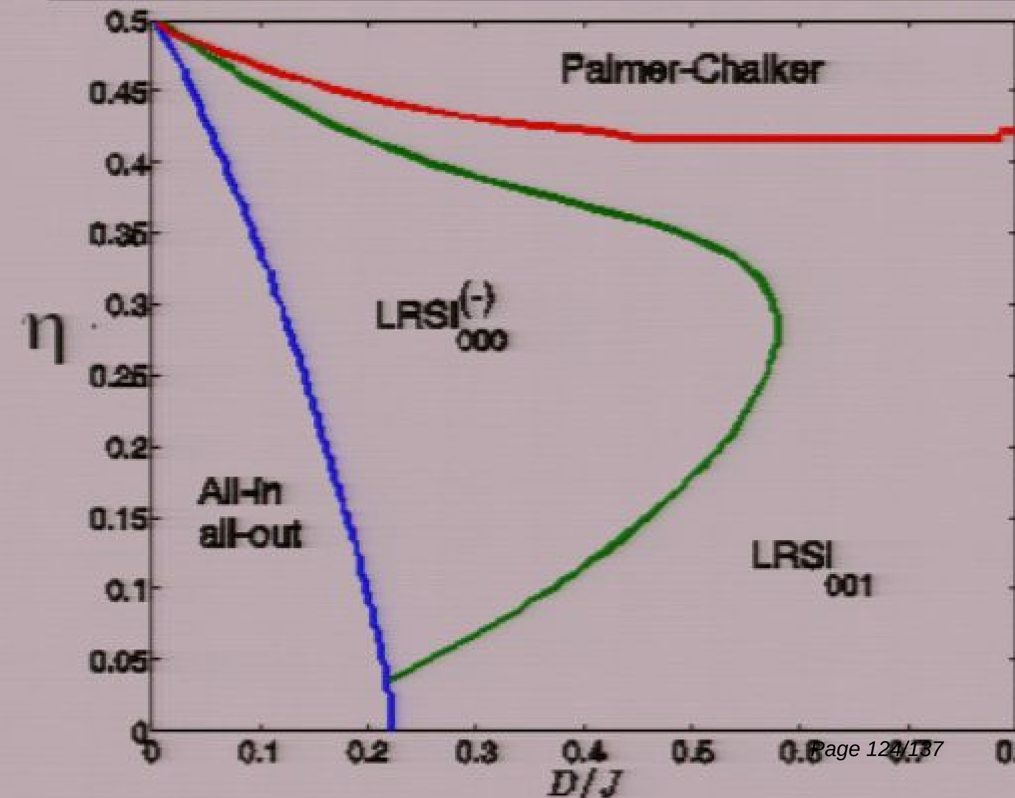
Simpler phenomenological model – not derived

$$H' = J_{ex}\sum_{\langle i,j\rangle}\vec{J}_i\bullet\vec{J}_j + DR_{nn}^3\sum_{\substack{i,j\\ j>i}}\left\{\frac{(\vec{J}_i\bullet\vec{J}_j)}{|\vec{R}_{ij}|^3}-\frac{3(\vec{J}_i\bullet\vec{R}_{ij})(\vec{R}_{ij}\bullet\vec{J}_j)}{|\vec{R}_{ij}|^5}\right\}$$

From H_{eff} derived from H_{micro}



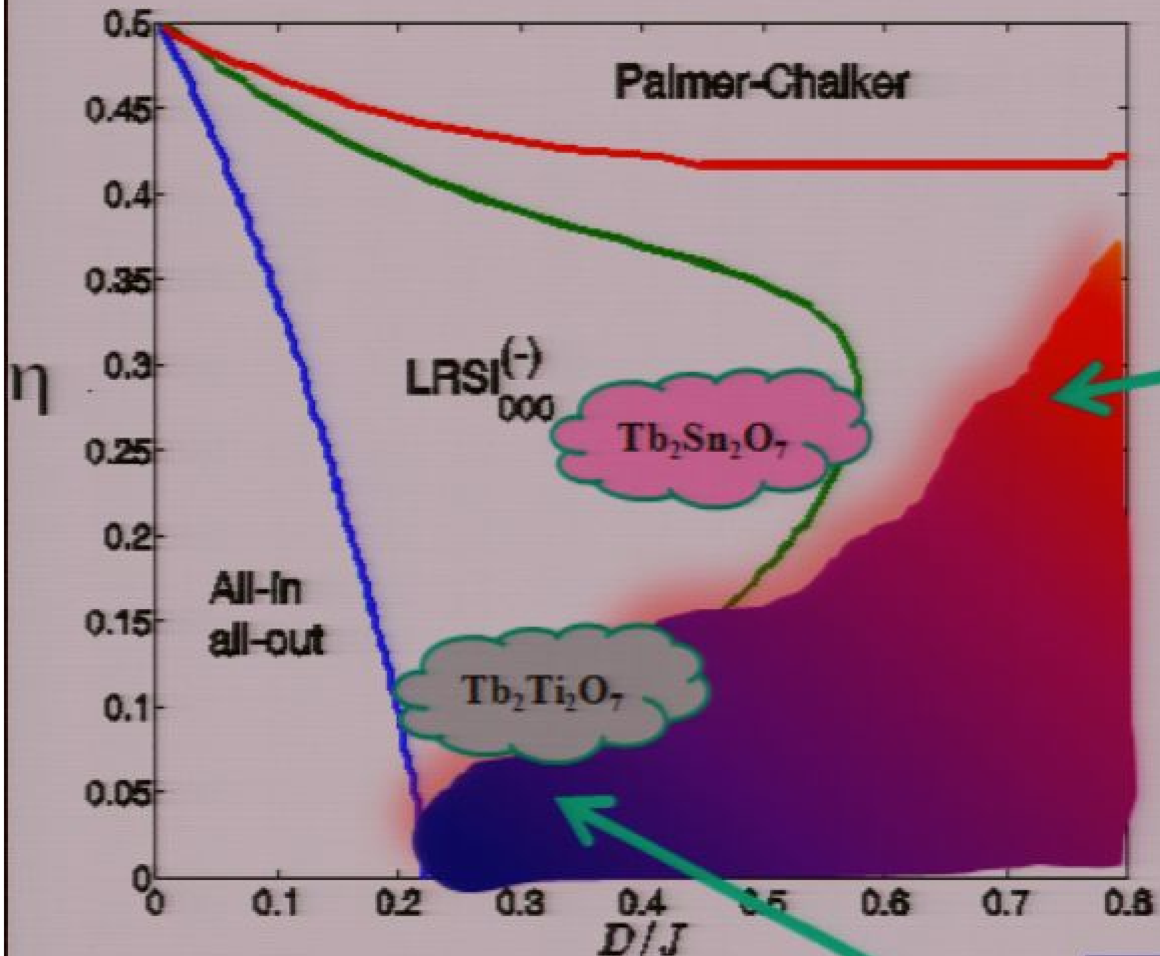
$H_{toy\text{-}model}$ not derived from H_{micro}



“Conclusion” about $Tb_2Ti_2O_7$ and $Tb_2Sn_2O_7$

- These materials are very interesting and show perplexing behaviors.
- $Tb_2Ti_2O_7$ is particularly interesting, being a rare example of a three-dimensional spin liquid.
- Maybe a “quantum spin ice”
- Could deviations from infinite Ising anisotropy make $Tb_2Ti_2O_7$ a possible material realizing exotic spin liquid properties such as emergent: U(1) gauge theory, emerging photons and deconfined & fractionalized spinons and monopoles?

Simpler phenomenological model



Can hardly reach that state when cooling from paramagnetic phase

Cannot reach that state when cooling from paramagnetic phase

Simpler phenomenological model – not derived

$$H' = H_{\text{ex}} + H_{\text{dip}}$$

$$H_{\text{ex}} = J_{\text{ex}} \sum_{\langle i,j \rangle} \vec{\mathrm{J}}_i \bullet \vec{\mathrm{J}}_j$$

$$H_{\text{dip}} = D R_{nn}^3 \sum_{\substack{i,j \\ j>i}} \left\{ \frac{(\vec{\mathrm{J}}_i \bullet \vec{\mathrm{J}}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{\mathrm{J}}_i \bullet \vec{R}_{ij})(\vec{R}_{ij} \bullet \vec{\mathrm{J}}_j)}{|\vec{R}_{ij}|^5} \right\}$$

$$\vec{\mathrm{J}}_i = \left(\eta S_i^{x_i}, \eta S_i^{y_i}, (1-\eta) S_i^{z_i} \right)$$

- η=0 : Ising limit
- η=1/2: Heisenberg limit
- η=1 : XY limit

Effective spin-1/2 (XXZ) model

$$V = J_{\text{ex}} \sum_{\langle i,j \rangle} \vec{J}_i \bullet \vec{J}_j + D R_{nn}^3 \sum_{\substack{i,j \\ j>i}} \left\{ \frac{(\vec{J}_i \bullet \vec{J}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{J}_i \bullet \vec{R}_{ij})(\vec{R}_{ij} \bullet \vec{J}_j)}{|\vec{R}_{ij}|^5} \right\}$$

$$H_{\text{eff}} = \sum_{i>j} J_{ij}^{z_i z_j} \left(r_{ij} \right) S_i^{z_i} S_j^{z_j} + \sum_{\substack{i>j \\ u \neq v \neq z}} J_{ij}^{u_i v_j} \left(r_{ij} \right) S_i^{u_i} S_j^{v_j}$$

pseudo spin-1/2 model

<u>But now, on the lattice, not only on a single tetrahedron</u>

Effective Hamiltonian Method

$$V = J_{ex}\sum_{\langle i,j\rangle}\vec{J}_i\bullet\vec{J}_j + DR_{nn}^3\sum_{\substack{i,j\\ j>i}}\left\{\frac{(\vec{J}_i\bullet\vec{J}_j)}{|\vec{R}_{ij}|^3}-\frac{3(\vec{J}_i\bullet\vec{R}_{ij})(\vec{R}_{ij}\bullet\vec{J}_j)}{|\vec{R}_{ij}|^5}\right\}$$

H_{ex} H_{dip}

$$H_{eff} = PVP + PVQVP + \cdots$$

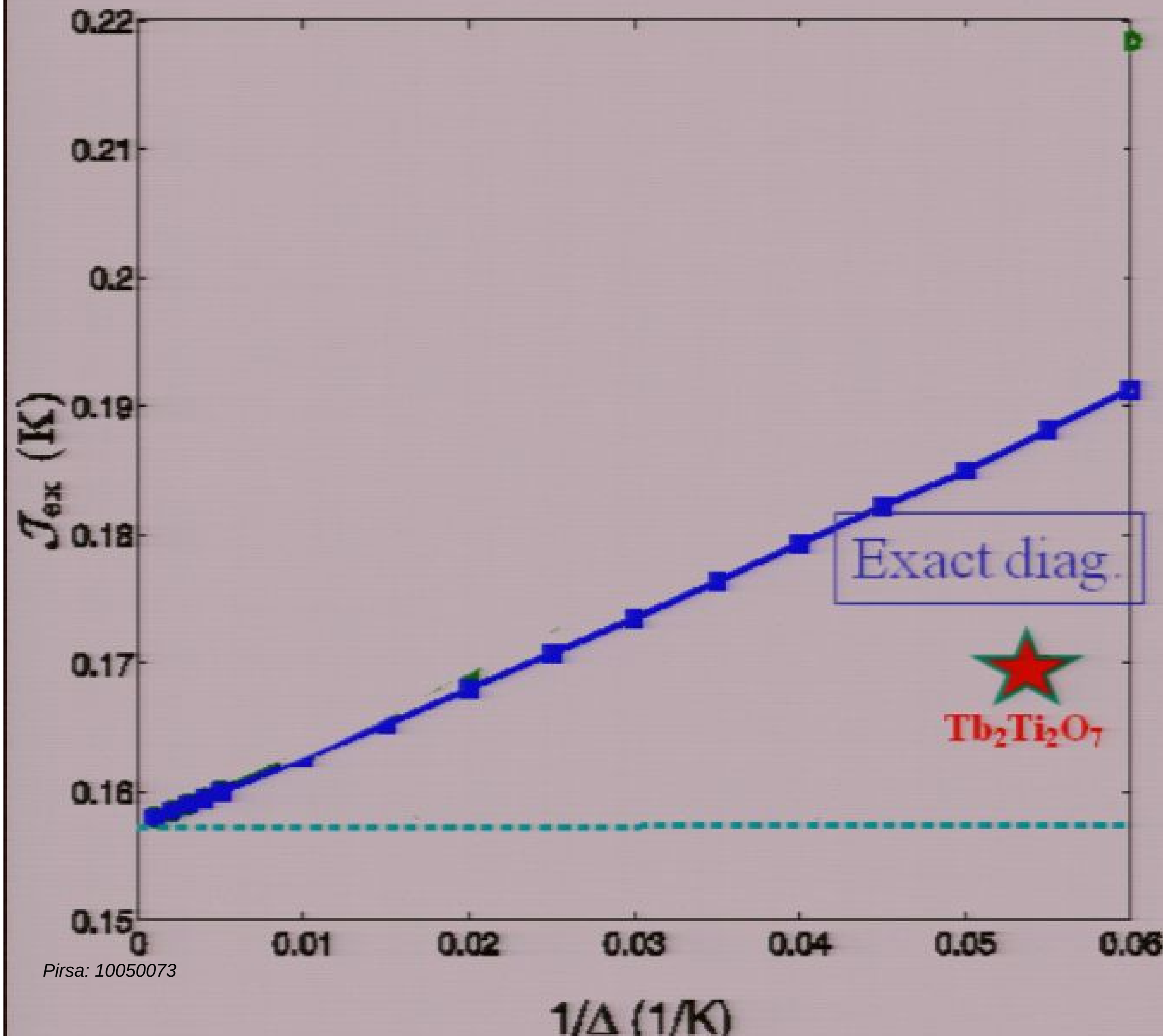
$$P = \sum_{\alpha\in P}|\alpha\rangle\langle\alpha|$$

Large denominator compared to the energy scale of H'

$$Q = \sum_{\beta\notin P}\frac{|\beta\rangle\langle\beta|}{E_0^\alpha - E_0^\beta}$$

$$H_{eff} = PH_{ex}P + PH_{dip}P + PH_{ex}QH_{ex}P$$
$$+(PH_{ex}QH_{dip}P + PH_{dip}QH_{ex}P) + PH_{dip}QH_{dip}P$$

Single tetrahedron phase diagram $Tb_2Ti_2O_7$



Effective Hamiltonian Method

$$V = J_{ex}\sum_{\langle i,j\rangle}\vec{J}_i\bullet\vec{J}_j + DR_{nn}^3\sum_{\substack{i,j\\ j>i}}\left\{\frac{(\vec{J}_i\bullet\vec{J}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{J}_i\bullet\vec{R}_{ij})(\vec{R}_{ij}\bullet\vec{J}_j)}{|\vec{R}_{ij}|^5}\right\}$$

H_{ex} $\quad$ H_{dip}

$$H_{eff} = PVP + PVQVP + \cdots$$

$$\mathbf{P} = \sum_{\alpha\in \mathbf{P}}|\alpha\rangle\langle\alpha|$$

$$Q = \sum_{\beta\notin P}\frac{|\beta\rangle\langle\beta|}{E_0^\alpha - E_0^\beta}$$

Effective Hamiltonian Method

$$V = J_{ex}\sum_{\langle i,j\rangle}\vec{J}_i \bullet \vec{J}_j + DR_{nn}^3 \sum_{\substack{i,j\\ j>i}}\left\{\frac{(\vec{J}_i \bullet \vec{J}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{J}_i \bullet \vec{R}_{ij})(\vec{R}_{ij} \bullet \vec{J}_j)}{|\vec{R}_{ij}|^5}\right\}$$

H_{ex} $\quad H_{dip}$

Effective Hamiltonian Method

$$V = J_{ex}\sum_{\langle i,j\rangle}\vec{\mathrm{J}}_i \bullet \vec{\mathrm{J}}_j + DR_{nn}^3 \sum_{\substack{i,j\\ j>i}}\left\{\frac{(\vec{\mathrm{J}}_i \bullet \vec{\mathrm{J}}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{\mathrm{J}}_i \bullet \vec{R}_{ij})(\vec{R}_{ij} \bullet \vec{\mathrm{J}}_j)}{|\vec{R}_{ij}|^5}\right\}$$

H_{ex} H_{dip}

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$$H_{\mathrm{eff}} = PH_{\mathrm{ex}}P + PH_{\mathrm{dip}}P + PH_{\mathrm{ex}}QH_{\mathrm{ex}}P$$
$$+(PH_{\mathrm{ex}}QH_{\mathrm{dip}}P + PH_{\mathrm{dip}}QH_{\mathrm{ex}}P) + PH_{\mathrm{dip}}QH_{\mathrm{dip}}P$$

Effective Hamiltonian Method

$$V = \underbrace{J_{ex} \sum_{\langle i,j \rangle} \vec{J}_i \bullet \vec{J}_j}_{H_{ex}} + \underbrace{DR_{nn}^3 \sum_{\substack{i,j \\ j>i}} \left\{ \frac{(\vec{J}_i \bullet \vec{J}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{J}_i \bullet \vec{R}_{ij})(\vec{R}_{ij} \bullet \vec{J}_j)}{|\vec{R}_{ij}|^5} \right\}}_{H_{dip}}$$

$$H_{eff} = PVP + PVQVP + \cdots$$

$$\mathbf{P} = \sum_{\alpha \in \mathbf{P}} |\alpha\rangle\langle\alpha|$$

Large denominator compared to the energy scale of H'

$$Q = \sum_{\beta \notin P} \frac{|\beta\rangle\langle\beta|}{E_0^\alpha - E_0^\beta}$$

$$H_{eff} = PH_{ex}P + PH_{dip}P + PH_{ex}QH_{ex}P$$
$$+(PH_{ex}QH_{dip}P + PH_{dip}QH_{ex}P) + PH_{dip}QH_{dip}P$$

Effective spin-1/2 (XXZ) model

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pseudo spin-1/2 model

Effective Hamiltonian Method

$$V = J_{ex} \sum_{\langle i,j \rangle} \vec{J}_i \bullet \vec{J}_j + DR_{nn}^3 \sum_{\substack{i,j \\ j>i}} \left\{ \frac{(\vec{J}_i \bullet \vec{J}_j)}{|\vec{R}_{ij}|^3} - \frac{3(\vec{J}_i \bullet \vec{R}_{ij})(\vec{R}_{ij} \bullet \vec{J}_j)}{|\vec{R}_{ij}|^5} \right\}$$

H_{ex} $\quad$ H_{dip}

$$H_{eff} = PVP + PVQVP + \cdots$$

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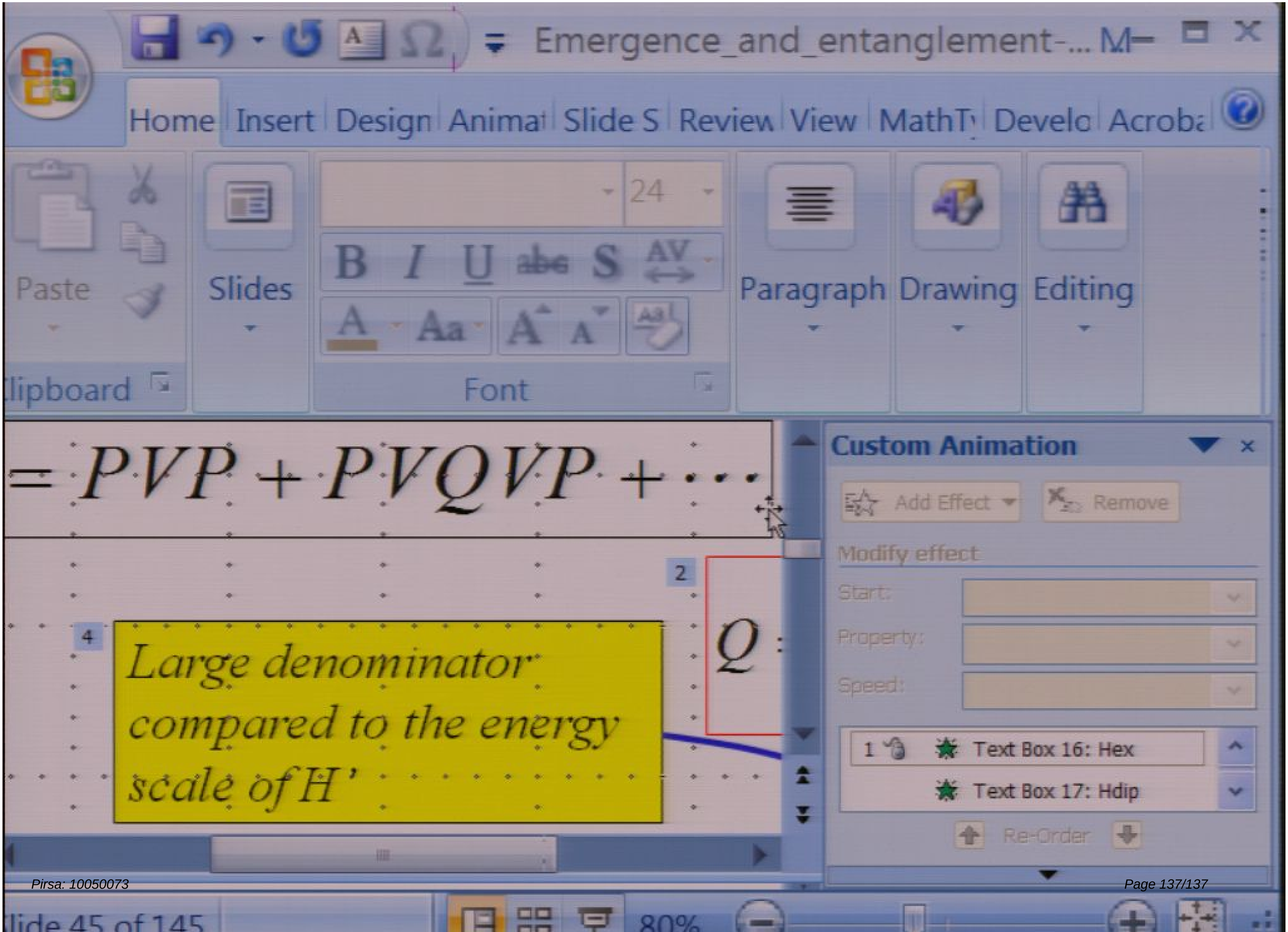
$$H_{eff} = PH_{ex}P + PH_{dip}P + PH_{ex}QH_{ex}P$$

$$+(PH_{ex}QH_{dip}P + PH_{dip}QH_{ex}P) + PH_{dip}QH_{dip}P$$


Emergence_and_entanglement-...
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Slides
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Drawing
Editing
Font
$= PVP + PVQVP + \cdots$
Large denominator compared to the energy scale of H'
Custom Animation
Add Effect
Remove
Modify effect
Start:
Property:
Speed:
Text Box 16: Hex
Text Box 17: Hdip
Re-Order
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80%