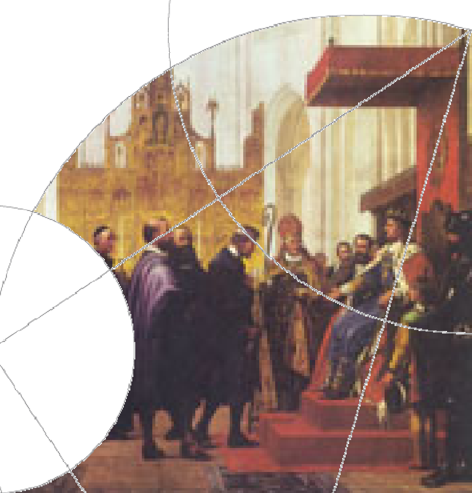
Bose-Einstein condensation — in the spin-dimer system $TlCuCl_3$(?)

Jens Jensen

in collaboration with
Henrik Smith

Henrik Smith symposium
Lundbeckfond Auditorium
27. November 2009



Background

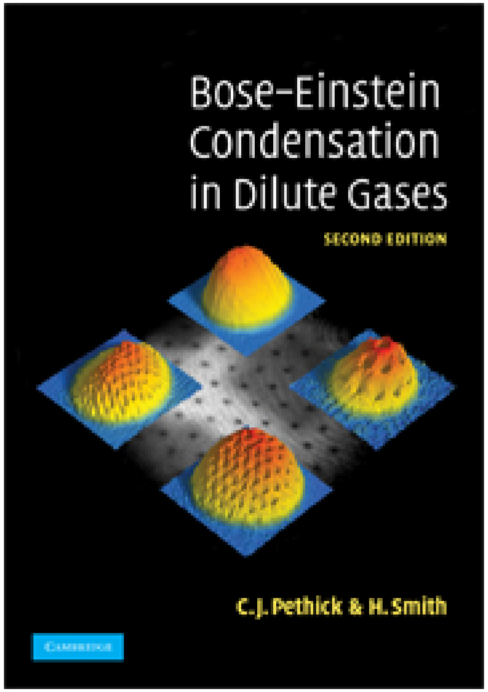
Kim Lefmann's "Magnetisme basisgruppe":

nature physics | VOL 4 | MARCH 2008 | www.nature.com/naturephysics

REVIEW ARTICLE | FOCUS

Bose–Einstein condensation in magnetic insulators

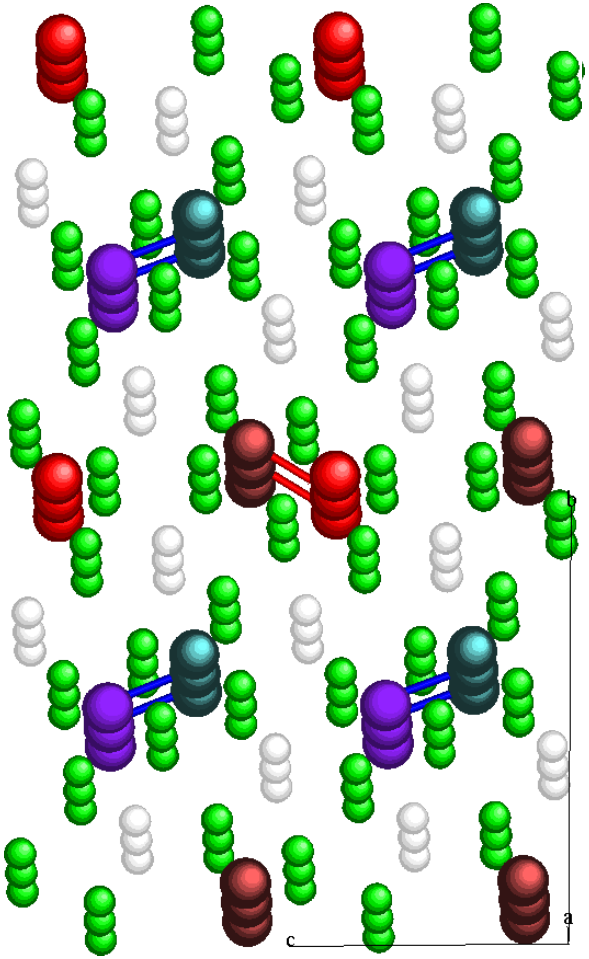
THIERRY GIAMARCHI[1]*, CHRISTIAN RÜEGG[2]* AND OLEG TCHERNYSHYOV[3]*



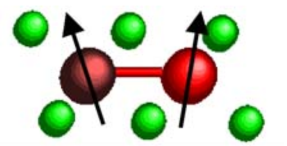
9. januar 2009:

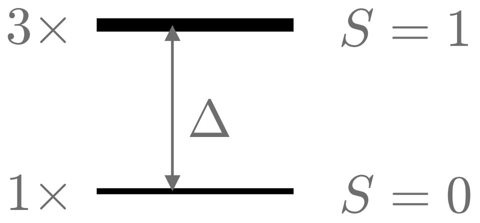
Henrik Smith om "Bose-Einstein kondensation i magnetiske systemer"

Crystal structure and “dimers” in $TlCuCl_3$



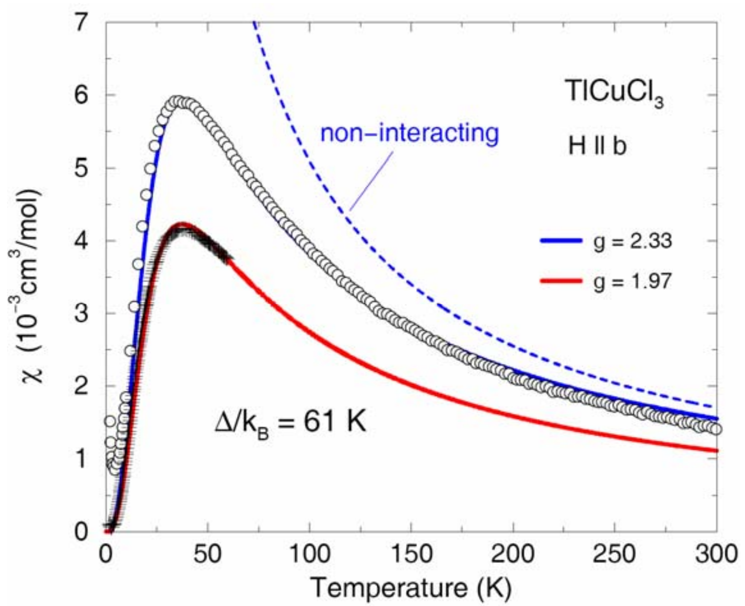
Monoclinic $P2_1/c$



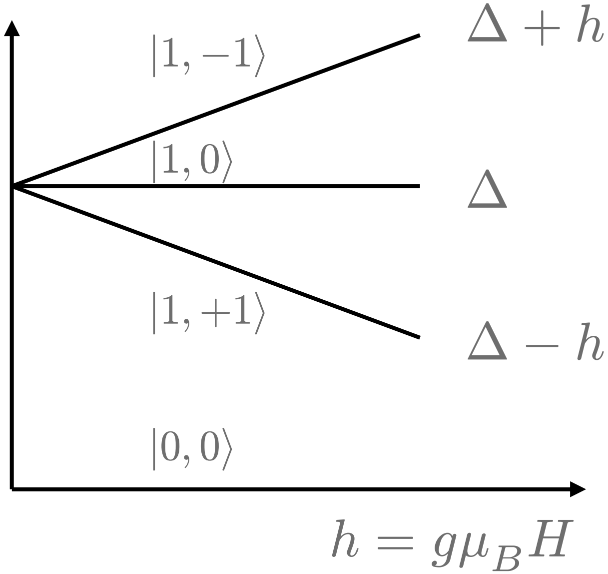


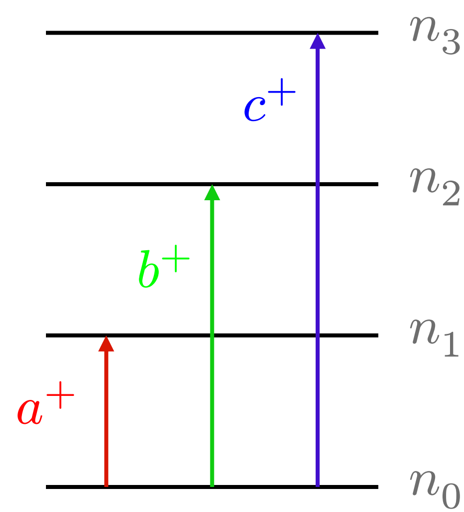
$$\vec{S} = \vec{s}_1 + \vec{s}_2$$

$$\mathcal{H} = \Delta\, \vec{s}_1 \cdot \vec{s}_2 = \frac{\Delta}{2}\left(\vec{S}^2 - \vec{s}_1{}^2 - \vec{s}_2{}^2\right)$$



Magnetic field and the excitations





$$a^+ = |1,+1\rangle\langle 0,0|$$
$$b^+ = |1,0\rangle\langle 0,0|$$
$$c^+ = |1,-1\rangle\langle 0,0|$$

Dimer-spin operators: $\vec{S} = \vec{s}_1 + \vec{s}_2$ and $\vec{\overline{S}} = \vec{s}_1 - \vec{s}_2$

$$\vec{S} \approx \vec{0}, \qquad \overline{S}_z = b + b^+, \quad \overline{S}_x = \frac{1}{\sqrt{2}}(c + c^+) - \frac{1}{\sqrt{2}}(a + a^+), \quad \overline{S}_y = \cdots$$

$$\mathcal{H} = \mathcal{H}_{\text{dimers}} + \mathcal{H}_{\text{exchange}}$$

$$\mathcal{H}_{\text{dimers}} = \sum_i \left[(\Delta - h)a_i^+ a_i + \Delta\, b_i^+ b_i + (\Delta + h)c_i^+ c_i\right]$$

$$\mathcal{H}_{\text{exchange}} = -\sum_{ij} J(ij)\left[a_i^+ a_j + b_i^+ b_j + c_i^+ c_j - a_i c_j - a_i^+ c_j^+ + \tfrac{1}{2}(b_i b_j + b_i^+ b_j^+)\right]$$

$$[a_i, a_i^+] = (|0,0\rangle\langle 0,0| - |1,+1\rangle\langle 1,+1|)_i \approx n_0 - n_1 = n_{01}$$

Magnetic excitations

Random Phase Approximation (RPA):

Longitudinal mode: $E^z_{\vec{q}} = \sqrt{\Delta^2 - 2\Delta n_{02} J(\vec{q})}$

Transverse modes (left and right handed circular polarization):

$$E^{\pm}_{\vec{q}} = \sqrt{\Delta^2 - \Delta(n_{01} + n_{03})J(\vec{q}) + (\tfrac{1}{2} n_{13} J(\vec{q}))^2} \pm \left[h - \tfrac{1}{2} n_{13} J(\vec{q})\right]$$

The fluctuation-dissipation theorem:
Response function $\Rightarrow$ Correlation function
Bose-like populations of the collective normal modes

In RPA $\frac{1}{N}\sum_{\vec{q}} \langle b^+_{\vec{q}} b^+_{-\vec{q}} \rangle = \langle b^+_i b^+_i \rangle = \langle (|1,0\rangle\langle 0,0||1,0\rangle\langle 0,0|)_i \rangle$ is non-zero.

Self-consistent RPA (including higher-order Green functions):
The dynamic parameters become renormalized

$$J(\vec{q}) \quad \rightarrow \quad J_\alpha(\vec{q}) = J(\vec{q}) - a_\alpha$$
$$\Delta \quad \rightarrow \quad \Delta_\alpha = \Delta + \tfrac{1}{2} \sum_{\gamma \neq \alpha} a_\gamma$$

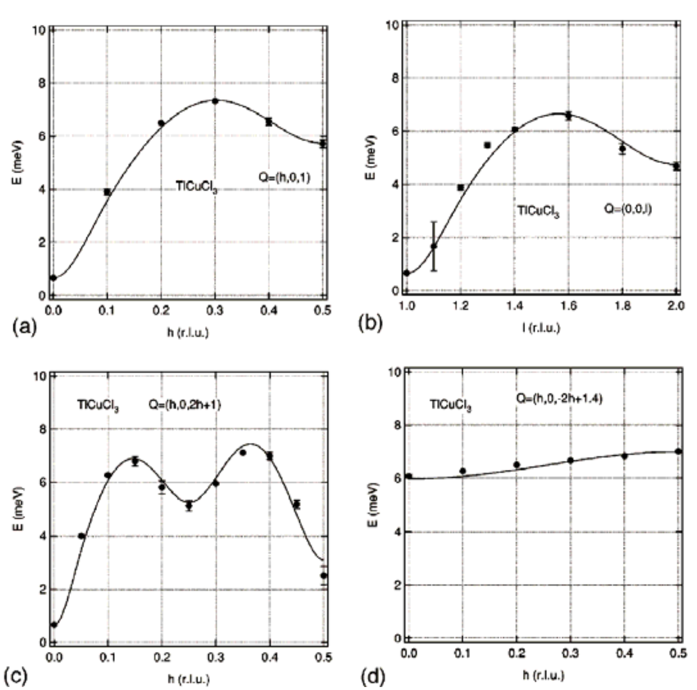
where a_z is determined so that $\langle b^+_i b^+_i \rangle = 0$

Magnetic excitations (II)

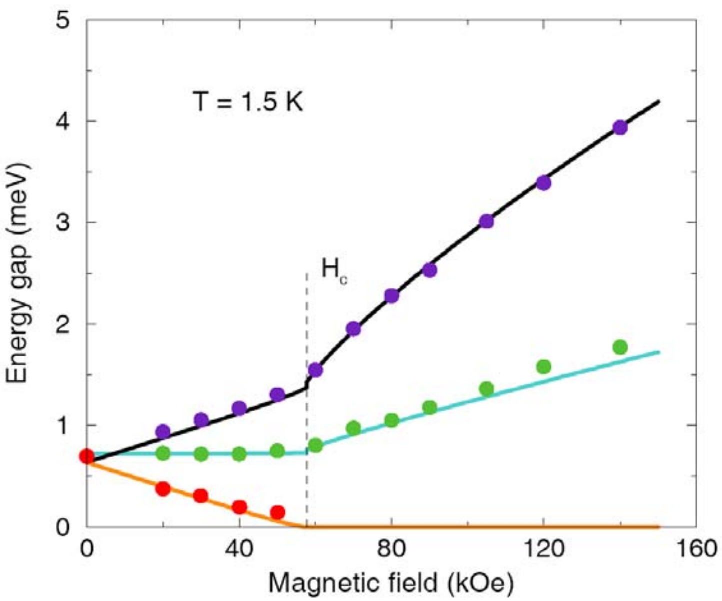
Longitudinal mode: $E^z_{\vec{q}} = \sqrt{\Delta_z^2 - 2\Delta_z n_{02} J_z(\vec{q})}$

Transverse modes ($n_{13} \approx 0$): $E^{\pm}_{\vec{q}} = \sqrt{\Delta_{\pm}^2 - 2\Delta_{\pm} n_{01} J_{\pm}(\vec{q})} \pm h$

$TlCuCl_3$ at $H = 0$ and $T = 1.5$ K

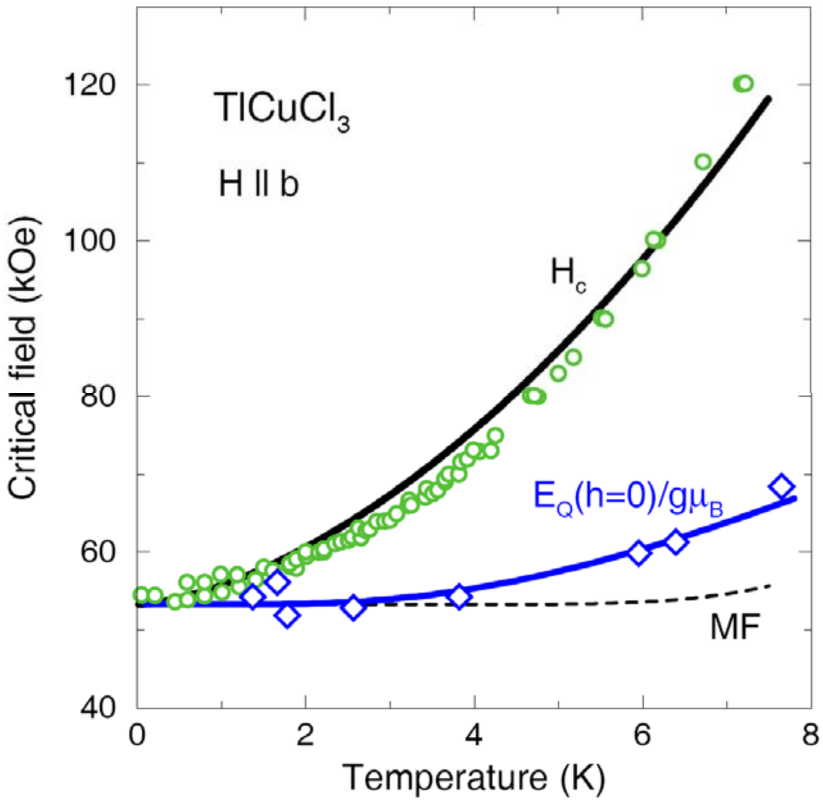


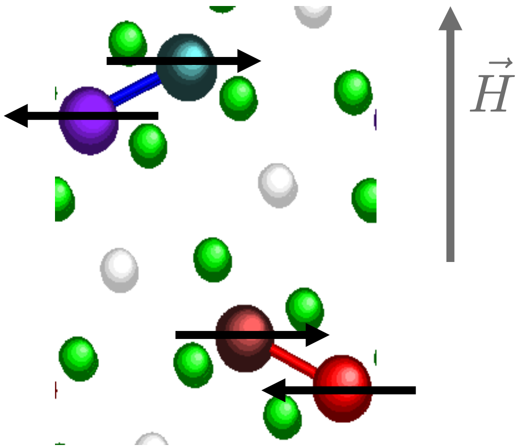
A. Oosawa *et al.*, Phys. Rev. B **65**, 094426 (2002).



C. Rüegg *et al.*, Appl. Phys. A **74**, S840 (2002).

Field-induced antiferromagnetic order





Order parameter:

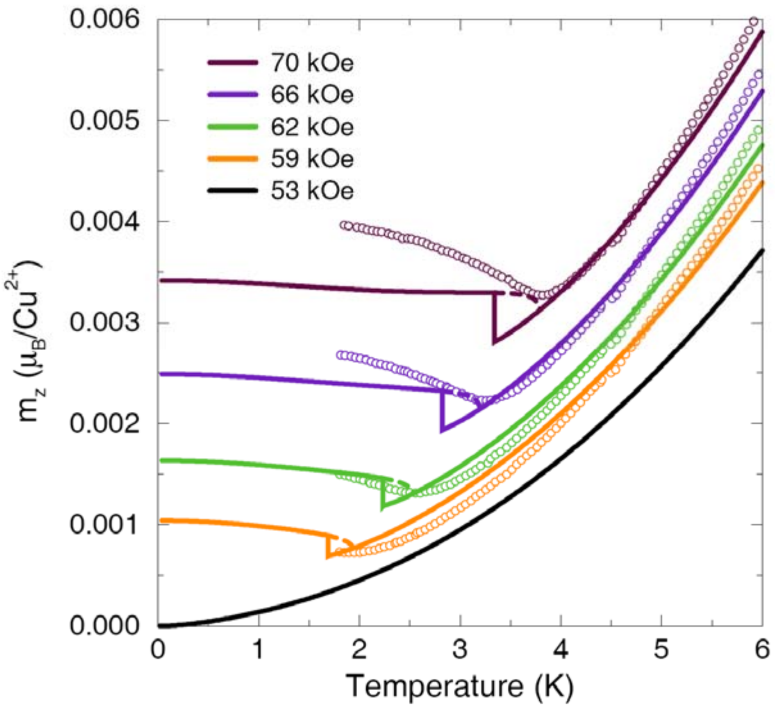
$$m_{xy} = \frac{1}{2} g\mu_B \langle \overline{S_x} \rangle$$

Induced bulk moment:

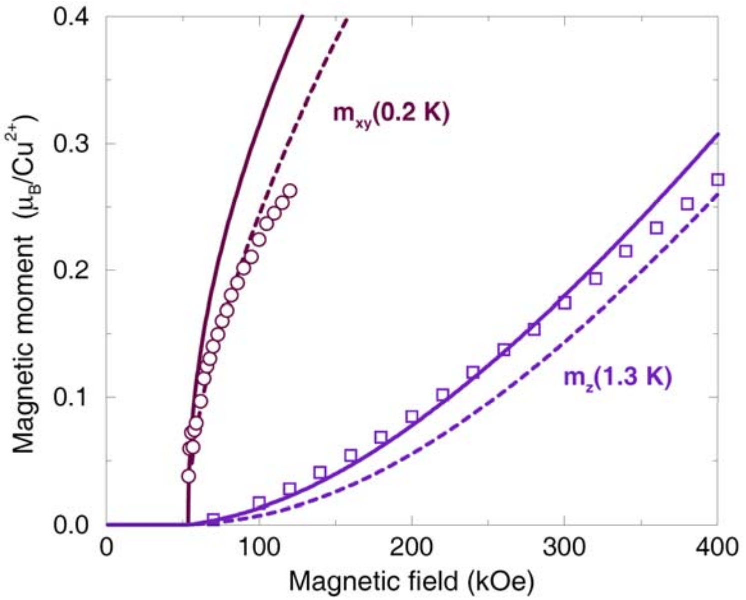
$$m_z = \frac{1}{2} g\mu_B \langle S_z \rangle$$

A. Oosawa *et al.*, Phys. Rev. B **63**, 134416 (2001).
Y. Shindo and H. Tanaka, J. Phys. Soc. Jpn **73**, 2642 (2004).
Ch. Rüegg *et al.*, Phys. Rev. Lett. **95**, 267201 (2005).

Magnetization curves



A. Oosawa *et al.*, J. Phys.: Condens. Matter **11**, 265 (1999).
T. Nikuni *et al.*, Phys. Rev. Lett. **84**, 5868 (2000).

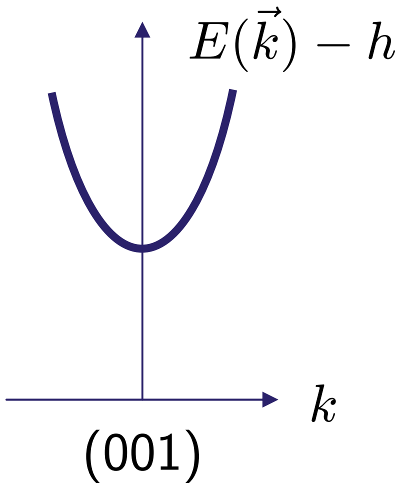


H. Tanaka *et al.*, J. Phys. Soc. Jpn. **70**, 939 (2001).
K. Tatani *et al.* published in Phys. Rev. B **69**, 054423 (2004).

$$m_z \approx \frac{H}{\Delta(n_{01} + n_{03})} m_{xy}^2$$

Effective Bose-particle model

T. Nikuni *et al.*, Phys. Rev. Lett. **84**, 5868 (2000).



$$\mathcal{H} = \sum_{\boldsymbol{k}} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} + \frac{v_0}{2} \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}} a^\dagger_{\boldsymbol{k}+\boldsymbol{q}} a^\dagger_{\boldsymbol{k}'-\boldsymbol{q}} a_{\boldsymbol{k}'} a_{\boldsymbol{k}}$$

where

$E(\vec{k}) \quad \Rightarrow \quad m$

$-\mu = E(001) - h$

v_0 is a free fitting parameter.

Magnetic soft-mode phase transition → Bose-Einstein Condensation

CONCLUSION

- The self-consistently renormalized RPA offers a coherent theory for the low-temperature properties of the $TlCuCl_3$ dimer system.
- The account of the paramagnetic properties is reasonable, whereas the description of the ordered phase is less satisfactory.
- The application of the more stringent diagrammatic 1/z-expansion theory is expected to improve on this circumstance, and it would allow an extension of the theory to higher temperatures, where damping effects become important.
- The magnetic ordering of a “singlet-ground state” system shows analogies with a “Bose-Einstein condensate”, however, the mapping of the magnetic Hamiltonian on the Bose-particle model is not well-defined (no prescription for how v_0 is determined).

**“Bose-Einstein condensation —
in the spin-dimer system $TlCuCl_3$”
is a questionable classification.**

Conclusion (digression)

PHYSICAL REVIEW B VOLUME 21, NUMBER 1 1 JANUARY 1980

Electrical resistivity of the singlet-ground-state system $Tb_cY_{1-c}Sb$

N. Hessel Andersen, J. Jensen, H. Smith, and O. Splittorff
Physics Laboratory I, H. C. Ørsted Institute, University of Copenhagen, Denmark

O. Vogt
Laboratorium für Festkörperphysik, ETH, Zurich, Switzerland
(Received 7 February 1979)

PHYSICAL REVIEW B ★★, ★★ (2010)

Bose–Einstein condensation and the magnetically ordered state of $TlCuCl_3$

Jens Jensen and Henrik Smith
Niels Bohr Institute, Universitetsparken 5, 2100 Copenhagen, Denmark
(Dated: October 23, 2009)

The dimerized $S = \frac{1}{2}$ spins of the Cu^{2+} ions in $TlCuCl_3$ are ordered antiferromagnetically in the presence of a field larger than about 54 kOe in the zero-temperature limit. Within the mean-field approximation all thermal effects are frozen out below 6 K. Nevertheless, experiments show significant changes of the critical field and the magnetization below this temperature, which reflect the presence of low-energetic dimer-spin excitations. We calculate the dimer-spin correlation functions within a self-consistent random-phase approximation, using as input the effective exchange coupling parameters obtained from the measured excitation spectra. The calculated critical field and magnetization curves exhibit the main features of those measured experimentally, but differ in important respects from the predictions of simplified boson models.