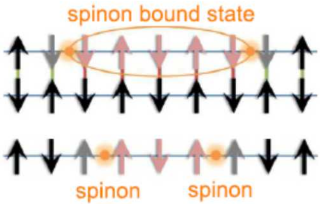
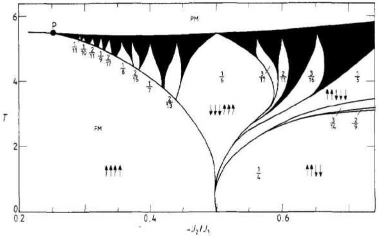
Ising model

Alexander Tsirlin

Experimentalphysik VI, Zentrum für elektronische Korrelationen und Magnetismus

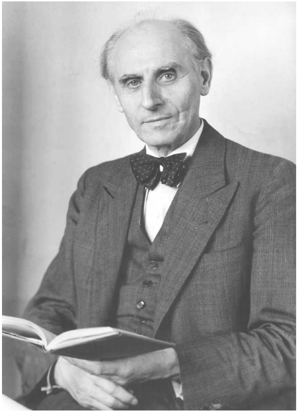




Alexander von Humboldt Stiftung/Foundation

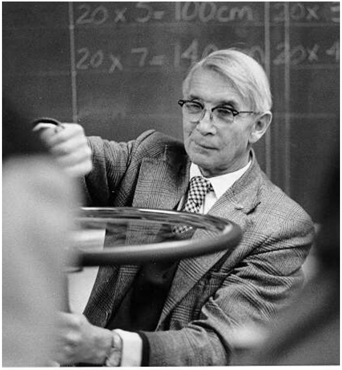
Theory of Magnetism, SS18

History of the Ising model



Wilhelm Lenz
1888–1957

First theory professor in Hamburg



Ernst Ising
1900–1998

Did teaching for most of his life
Germany till 1938, US since 1947

Origin of the Ising model

In a quantum treatment certain angles α will be distinguished, among them in any case $\alpha = 0$ and $\alpha = \pi$. If the potential energy W has large values in the intermediate positions, as one must assume taking account of the crystal, then these positions will be very seldom occupied, Umklapp processes will therefore occur very rarely, and the magnet will find itself in the two distinguished positions.

If one assumes that in the ferromagnetic bodies the potential energy of an atom (elementary magnet) with respect to its neighbors is different in the null position and in the π position, then there arises a natural directedness of the atom corresponding to the crystal state, and hence a spontaneous magnetization.

Wilhelm Lenz, Physikalische Zeitschrift 21, 613 (1920)

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Wilhelm Lenz, Physikalische Zeitschrift 21, 613 (1920)

Beitrag zur Theorie des Ferromagnetismus [1]).

Von **Ernst Ising** in Hamburg.

(Eingegangen am 9. Dezember 1924.)

Es wird im wesentlichen das thermische Verhalten eines linearen, aus Elementarmagneten bestehenden Körpers untersucht, wobei im Gegensatz zur Weissschen Theorie des Ferromagnetismus kein molekulares Feld, sondern nur eine (nicht magnetische) Wechselwirkung benachbarter Elementarmagnete angenommen wird. Es wird gezeigt, daß ein solches Modell noch keine ferromagnetischen Eigenschaften besitzt und diese Aussage auch auf das dreidimensionale Modell ausgedehnt.

E. Ising, Z. Phys. 31, 253 (1925)

Fate of the Ising model

- **1925, Ising:** no magnetic transition in 1D; could not solve the model in higher dimensions, but conjectured that the result should remain the same

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- **1932, Van Vleck:**
  In a certain sense the Lenz-Ising model is a purely mathematical fiction, as it neglects the interactions $-2J(s_i^x s_j^x + s_i^y s_j^y)$ between the components of spin perpendicular to the direction of the magnetic field, which are often important physically. The result should not be identified too closely with the actual magnetic behavior of the material simply because of the inadequacy and arbitrariness of the model.

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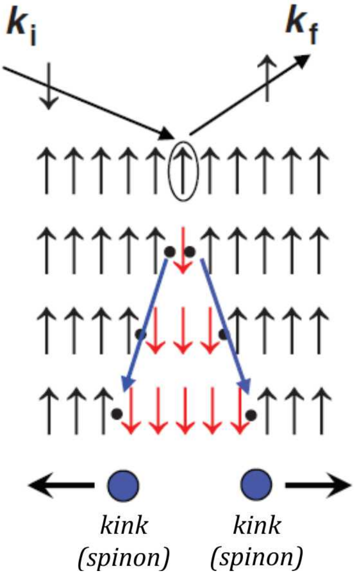
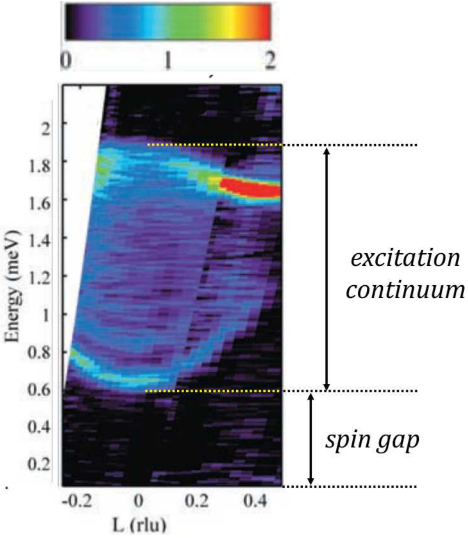
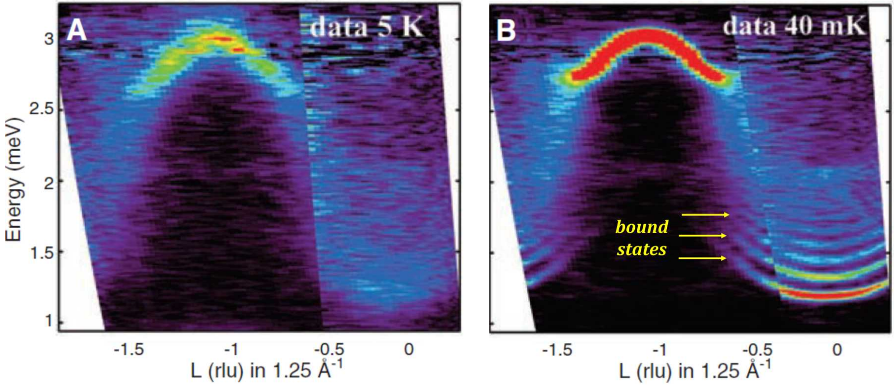
- Till 1950's: Ising model is a purely mathematical game
- Since 1960's: limited applications to rare-earth compounds
- Since $\sim$ 2000: deliberate search for Ising magnets





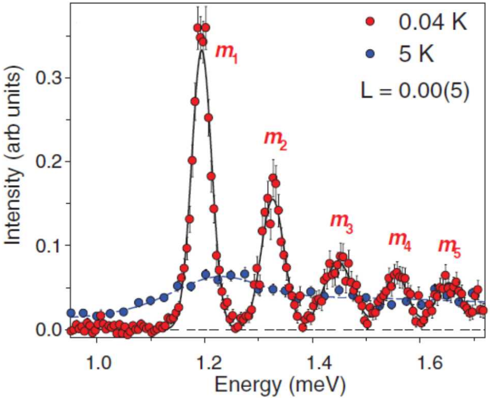
R. Coldea *et al.* Science 327, 177 (2010)

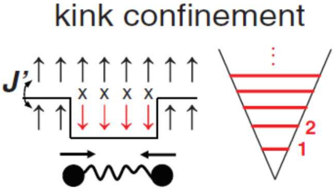


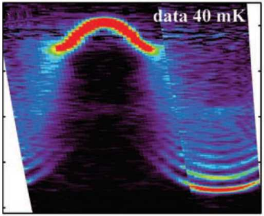
Free spinons | Bound spinons

- Excitation continuum splits into narrow excitations at low temperatures

R. Coldea *et al.* Science 327, 177 (2010)



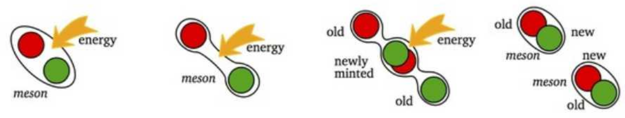


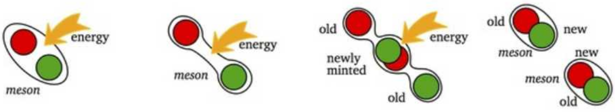


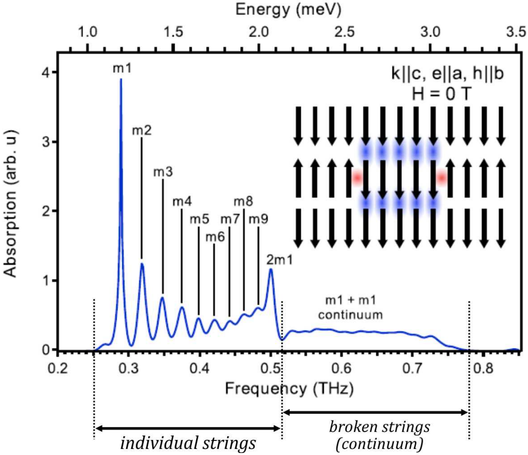
- Interchain interactions create an effective field
- Domains walls are bound in this effective potential and form a sequence of **bound states**

R. Coldea *et al.* Science 327, 177 (2010)

Confinement in particle physics



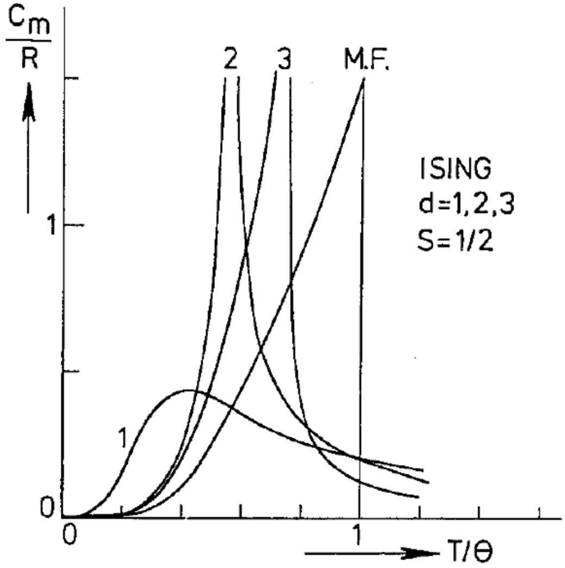




A string of two spinons can break into two strings with two spinons each

Equivalent to quark-antiquark pairs in hadrons (*quark confinement*)

C.M. Morris *et al.* Phys. Rev. Lett. 112, 137403 (2014)



Mean-field

Transition in any dimension

Finite jump of C_m at T_c

Exact

No transition in 1D

$T_c\,(3D) > T_c\,(2D)$

C_m diverges at T_c

L.J. de Jongh
and A.R. Miedema
Adv. Phys. 23, 1 (1974)

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  Did not manage (and did not try) to solve the model, but demonstrated non-zero magnetization at low temperatures, i.e., the formation of an ordered state in 2D

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  Approximate calculation of the partition function beyond mean field

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  Approximate calculation of the partition function beyond mean field

$$\mathfrak{A} = \begin{pmatrix}
0 & -2^{\frac12}k^{-2} & -2k^{-2} & -2^{\frac12}k^{-2} & -2k^{-2} & 0 & -2k^{-2} & -2^{\frac12}k^{-2} & -2k^{-2} & 0 & 0 & 0 & -2k^{-2} & 0 & -2k^{-2} & -2^{\frac12}k^{-2} \\
2^{\frac12}k^{-2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2^{\frac12}k^{-2} & -2 & 0 & -2 & -2^{\frac12}k^{-2} & -2 & -2^{\frac12}k^{-2} & 0 \\
2k^{-2} & 0 & 0 & 0 & 0 & 0 & 0 & 2^{\frac12}k^{-2} & 0 & -2^{\frac12}k^{2} & -2k^{2} & -2^{\frac12}k^{2} & 0 & 0 & 0 & -2^{\frac12}k^{-2} \\
2^{\frac12}k^{-2} & 0 & 0 & 0 & -2^{\frac12}k^{-2} & -2 & -2^{\frac12}k^{-2} & 0 & 2^{\frac12}k^{-2} & 2 & 0 & 2 & 0 & 0 & 0 & 0 \\
2k^{-2} & 0 & 0 & 2^{\frac12}k^{-2} & 0 & -2^{\frac12}k^{2} & 0 & -2^{\frac12}k^{-2} & 0 & 0 & -2k^{2} & -2^{\frac12}k^{2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2 & 2^{\frac12}k^{2} & 0 & 0 & -2 & 2^{\frac12}k^{2} & 0 & -2^{\frac12}k^{2} & 0 & -2^{\frac12}k^{2} & 0 & 0 & 2 \\
2k^{-2} & 0 & 0 & 2^{\frac12}k^{-2} & 0 & 0 & 0 & 0 & 0 & 0 & 2k^{2} & 2^{\frac12}k^{2} & 0 & -2^{\frac12}k^{2} & 0 & -2^{\frac12}k^{-2} \\
2^{\frac12}k^{-2} & 0 & -2^{\frac12}k^{-2} & 0 & 2^{\frac12}k^{-2} & 2 & 0 & 0 & 0 & 0 & 0 & -2 & 2^{\frac12}k^{-2} & 2 & 0 & 0 \\
2k^{-2} & 2^{\frac12}k^{-2} & 0 & -2^{\frac12}k^{-2} & 0 & -2^{\frac12}k^{2} & 0 & 0 & 0 & 0 & -2k^{2} & 0 & 0 & -2^{\frac12}k^{2} & 0 & 0 \\
0 & 2 & 2^{\frac12}k^{2} & -2 & 0 & 0 & 0 & 0 & 0 & 0 & -2^{\frac12}k^{2} & 0 & 2^{\frac12}k^{2} & 0 & -2^{\frac12}k^{2} & 2 \\
0 & 0 & 2k^{2} & 0 & 2k^{2} & 2^{\frac12}k^{2} & -2k^{2} & 0 & 2k^{2} & 2^{\frac12}k^{2} & 0 & -2^{\frac12}k^{2} & -2k^{2} & -2^{\frac12}k^{2} & 2k^{2} & 0 \\
0 & 2 & 2^{\frac12}k^{2} & -2 & 2^{\frac12}k^{2} & 0 & -2^{\frac12}k^{2} & 2 & 0 & 0 & 2^{\frac12}k^{2} & 0 & 0 & 0 & 0 & 0 \\
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0 & 2 & 0 & 0 & 0 & 0 & 2^{\frac12}k^{2} & -2 & 2^{\frac12}k^{2} & 0 & 2^{\frac12}k^{2} & 0 & 0 & 0 & -2^{\frac12}k^{2} & 2 \\
2k^{-2} & 2^{\frac12}k^{-2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2^{\frac12}k^{2} & -2k^{2} & 0 & 0 & 2^{\frac12}k^{2} & 0 & -2^{\frac12}k^{-2} \\
2^{\frac12}k^{-2} & 0 & 2^{\frac12}k^{-2} & 0 & 0 & -2 & 2^{\frac12}k^{-2} & 0 & 0 & -2 & 0 & 0 & 0 & -2 & 2^{\frac12}k^{-2} & 0
\end{pmatrix} \quad (69)$$

Lars Onsager
1903–1976

1968 Nobel prize in chemistry

for his discovery of the reciprocal relations bearing his name, which are fundamental for the thermodynamics of irreversible processes

> However, those who know him will witness the fact that he is clarity itself, and often responds at great length if the questions presented to him refer to *Norse mythology*, *gardening*, the more subtle aspects of *Kriegspiel* (a form of blindfold chess involving two opponents and a referee), and even encyclopedic facts of organic chemistry
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> Elliott Montroll

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Elliott Montroll

- 1942: exact partition function announced on a conference
- 1944: first publication
- 1947: human-readable publication (thanks to Onsager's PhD student)

$$\log \lambda_\infty = \tfrac{1}{2} \log(2 \sinh 2H) + \frac{1}{2\pi} \int_0^\pi \gamma(\omega) d\omega \quad (106)$$

where

$$\cosh \gamma(\omega) = \cosh 2H' \cosh 2H^* - \sinh 2H' \sinh 2H^* \cos \omega.$$

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Solution for the magnetization

- 1948: announced on a conference, never published
- 1952: published by C.N. Yang (following Onsager's advice)

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After Onsager

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Elliott Montroll

Hendrik Casimir (stayed in Netherlands throughout WWII):
What are the news in theoretical physics since 1940?

Wolfgang Pauli (worked in the US)
Nothing special, really, but Onsager's solution was an interesting piece of work

per Elliott Montroll

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per Elliott Montroll

Young physicists today may find it surprising, even unbelievable, that in the 1950's the Lenz-Ising model and similar problems were not deemed important by most physicists. They were considered arcane exercises, narrowly interesting, mathematically seducing, but of little real consequence.

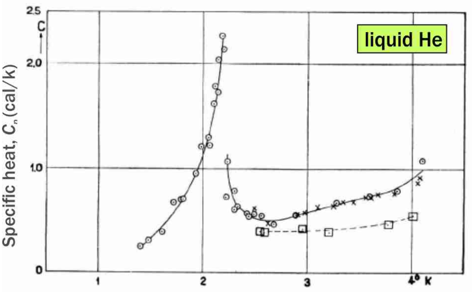
C.N. Yang

In the best mathematical tradition, not being able to solve the original problem,
I looked around for a similar problem which I could solve

Mark Kac about his attempted work on the Ising model in 3D

Paul Ehrenfest
1880–1933

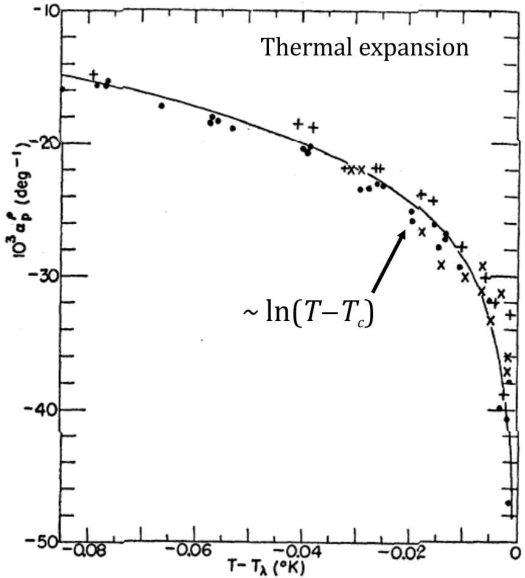
first theory of phase transitions



Superfluid transition of helium (λ-transition)
first example of a second-order transition

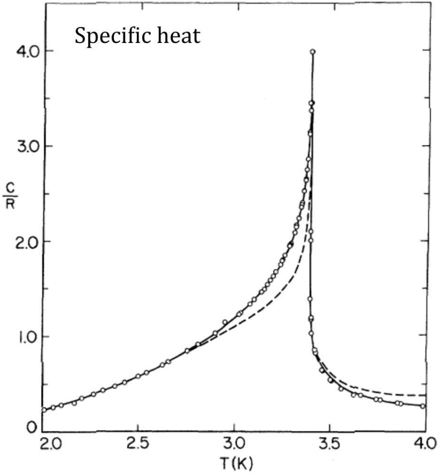
W.H. Keesom and K. Clusius,
KNAW Proceedings 35, 307 (1932)

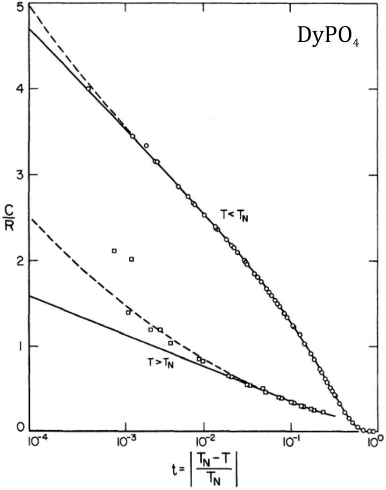
- **First order:** latent heat, discontinuity in $dF/d\alpha$
- **Second order:** no latent heat, discontinuity only in $d^2F/d\alpha^2$



λ-transition in He

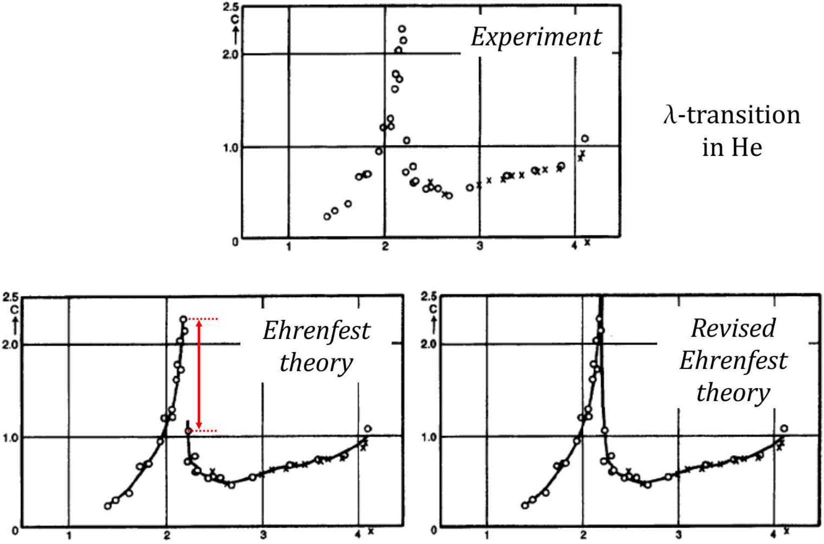
K.R. Atkins and M.H. Edwards
Phys. Rev. 97, 1429 (1955)





λ-type anomaly at the magnetic transition

J.C. Wright *et al.*
Phys. Rev. B 3, 843 (1971)



λ-transition in He

G. Jaeger, Arch. Hist. Exact. Sci. 53, 51 (1998)

Continuous transitions (former "second-order")

- First derivatives of the free energy ($dF/d\alpha$) change continuously
- Second derivatives ($d^2F/d\alpha^2$) may or may not have discontinuities
- No latent heat, no hysteresis
- Order parameter can be defined
- Constrained by symmetry (the transition follows one of the irreducible representations of the symmetry group)
- Examples:

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Discontinuous transitions (former "first-order")

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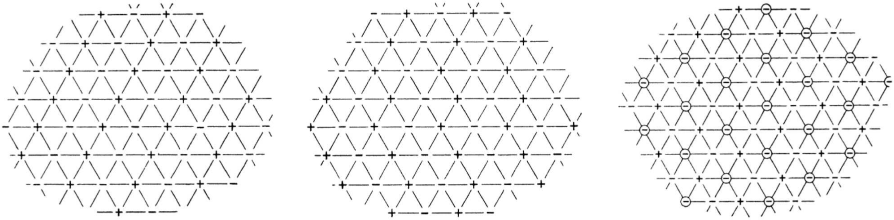
Discontinuous transitions (former "first-order")

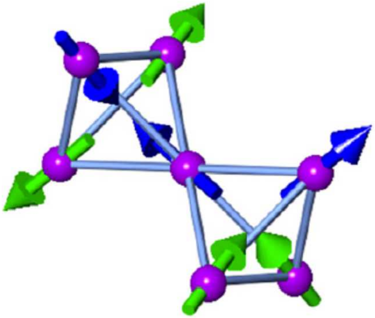
- First derivatives of the free energy ($dF/d\alpha$) show discontinuities
- Latent heat, hysteresis
- Examples: boiling/crystallization, magnetic ordering with a structural component

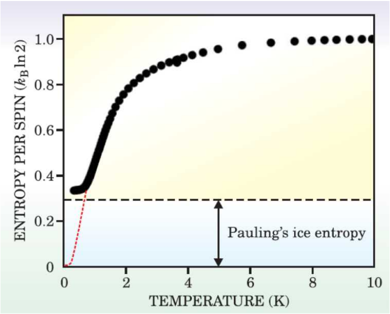


G. Wannier, Phys. Rev. 79, 357 (1950)

Antiferromagnetic Ising model on the triangular lattice

- Infinite number of configurations with the same energy (extensive ground-state degeneracy)
- Large residual entropy of $0.3383R$ (entropy at $T = 0$) nearly 50% of the total entropy of $R \ln 2$
- Violates the third law of thermodynamics





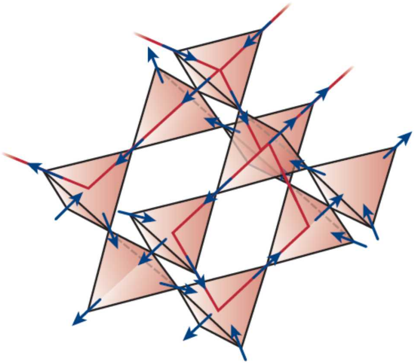
2-in-2-out states

infinite number of configurations possible

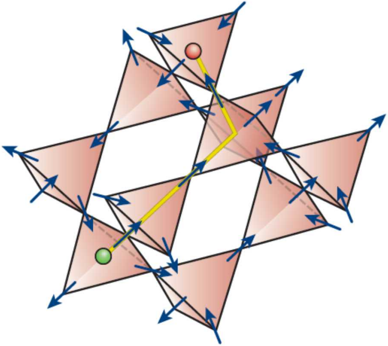
Residual entropy

(same as in water ice)

M.J.P. Gingras and P.A. McClarty, Rep. Prog. Phys. 77, 056501 (2014)
R. Moessner and A.P. Ramirez, Physics Today (2) 24 (2006)



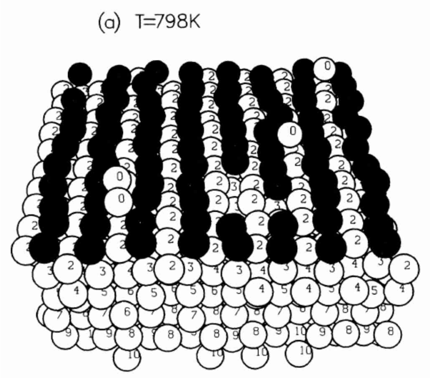
2-in-2-out configuration
(ground state)

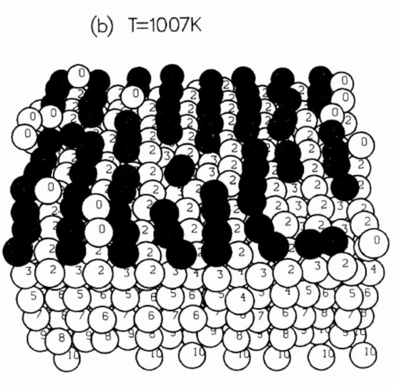


3-in-1-out + 1-in-3-out
(excitation)

- The tetrahedra with excited configurations (3-in-1-out and 1-in-3-out) can be viewed as **magnetic monopoles**

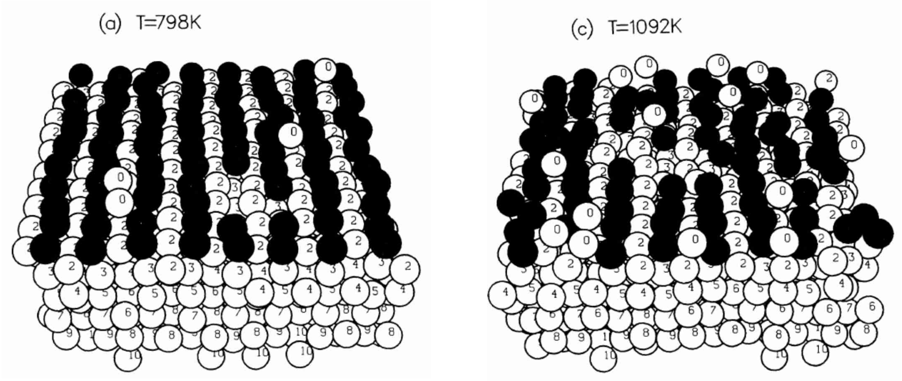
L. Balents, Nature 464, 199 (2010)
per C. Castelnovo *et al.* Nature 451, 42 (2008)





- Adsorbates form different phases (liquid or crystalline with different periodicity) depending on temperature and "field" (surface coverage)
- Relevant to catalysis, environmental research, etc.

H. Häkkinen and M. Manninen, Phys. Rev. B 46, 1725 (1992)



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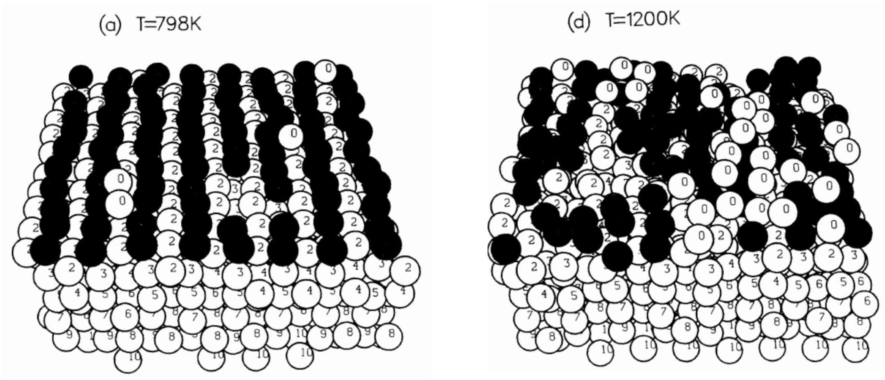
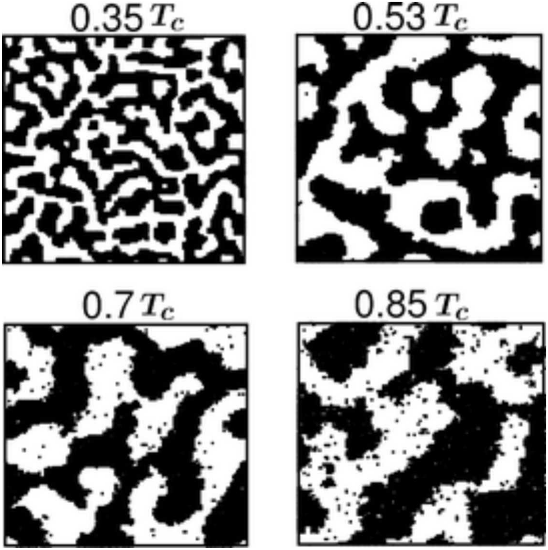
H. Häkkinen and M. Manninen, Phys. Rev. B 46, 1725 (1992)

Lattice gas models and absorption



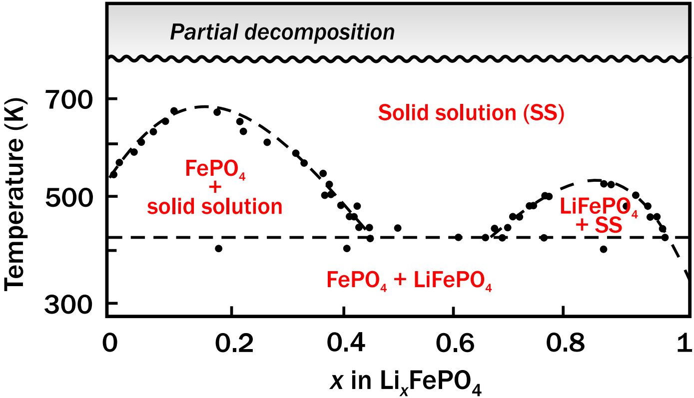
- Adsorbates form different phases (liquid or crystalline with different periodicity) depending on temperature and "field" (surface coverage)
- Relevant to catalysis, environmental research, etc.

H. Häkkinen and M. Manninen, Phys. Rev. B 46, 1725 (1992)

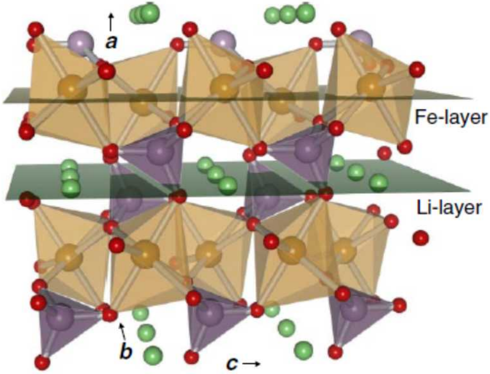


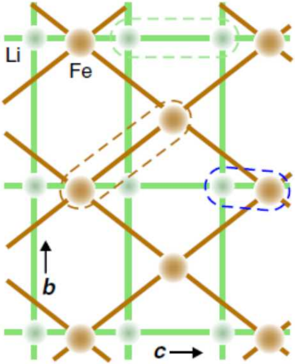
Binary alloy
after quenching to
temperatures below T_c

S. Majumder and S.K. Das, Phys. Chem. Chem. Phys. 15, 13209 (2013)



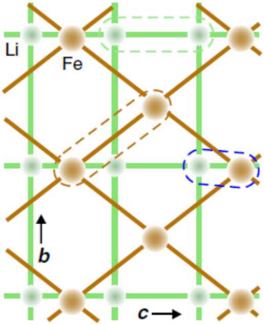
F. Zhou *et al.* Phys. Rev. Lett. 97, 155704 (2006)

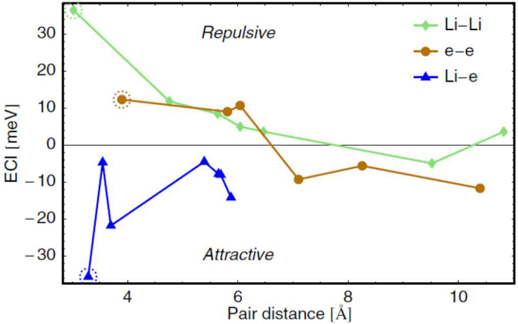




- Two ingredients:
  - Li atoms and vacancies
  - Additional electrons on Fe (2+ vs. 3+)
- Both Li-Li, $e - e$, and $Li - e$ interactions should be considered

F. Zhou *et al.* Phys. Rev. Lett. 97, 155704 (2006)





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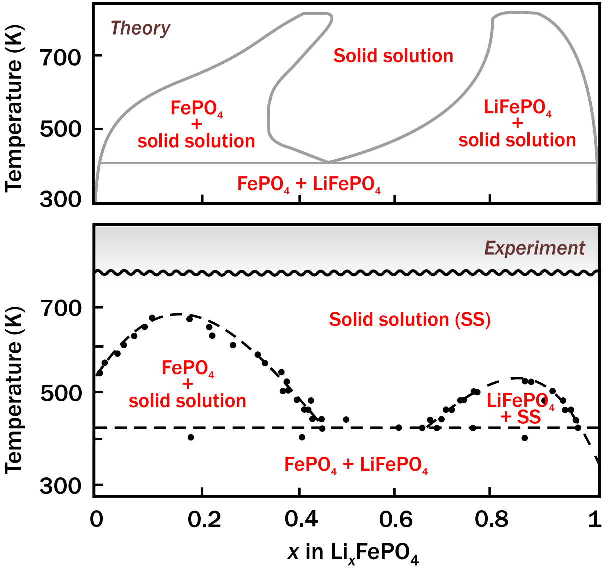
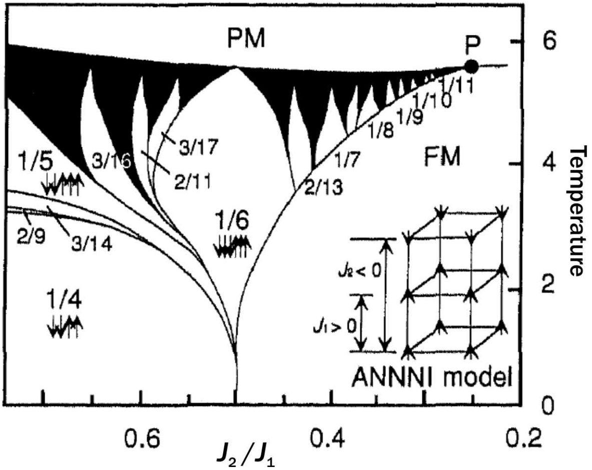
F. Zhou *et al.* Phys. Rev. Lett. 97, 155704 (2006)



All features of
the experimental
phase diagram
are captured
by the Ising model

F. Zhou *et al.*
Phys. Rev. Lett.
97, 155704 (2006)

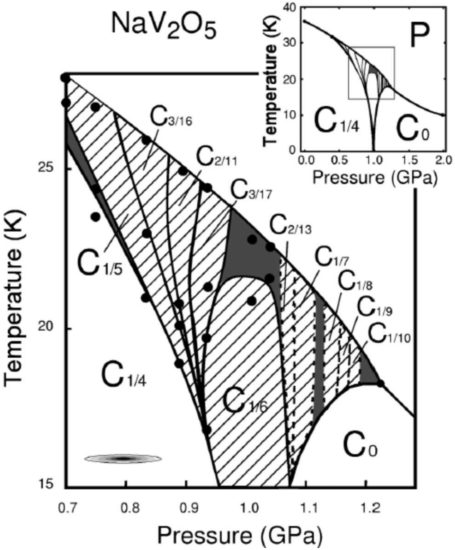


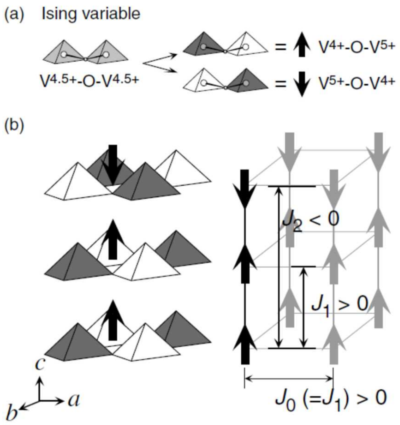
White areas:
commensurate order
($\frac{1}{4}$, $\frac{1}{8}$, $\frac{2}{11}$, etc.)

Dark areas:
incommensurate order
(period is not a simple rational number)

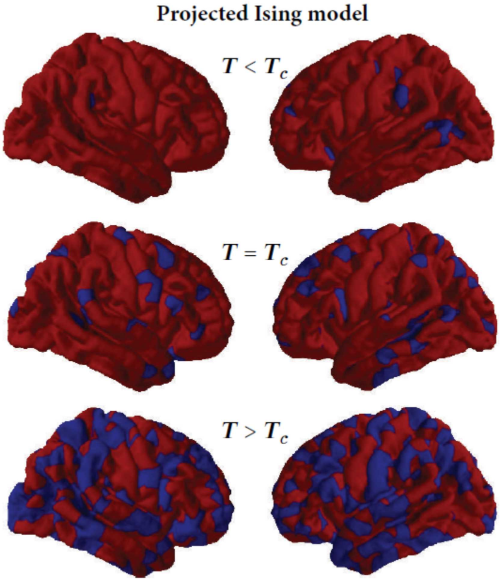
- ANNNI = anisotropic next-nearest-neighbor Ising model

K. Ohwada *et al.* Mod. Phys. Lett. B 20, 199 (2006)





K. Ohwada *et al.* Phys. Rev. Lett. 87, 086402 (2001)



Neuron activity represented by an Ising variable

T.K. Das *et al.* BioMed Research International 237898 (2014)

Applications in sociology

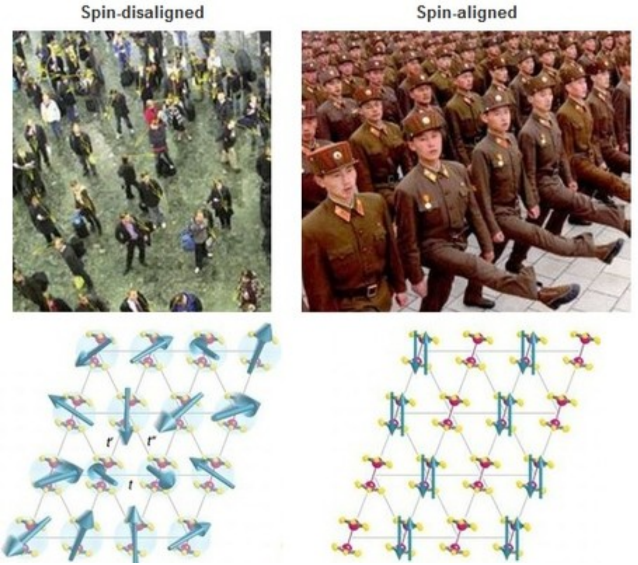
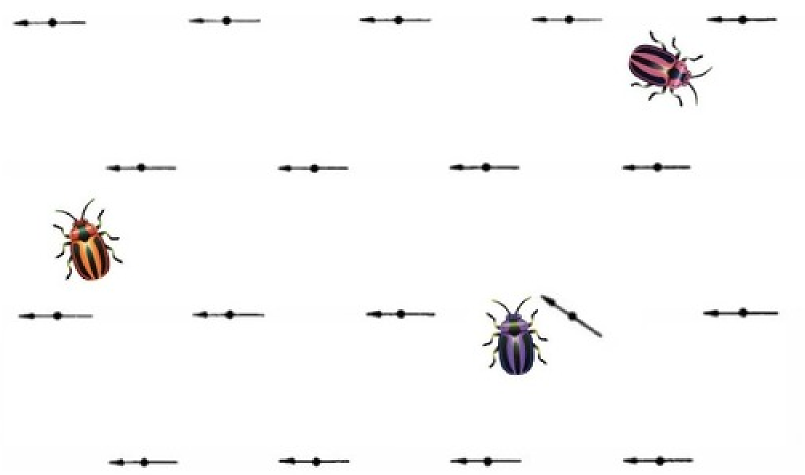


Image credit: eoht.info



V. Daniel, Sociological Review 44, 107 (1952)

Why Monte-Carlo?

Image credit: Martinp1 (Wikimedia Commons)

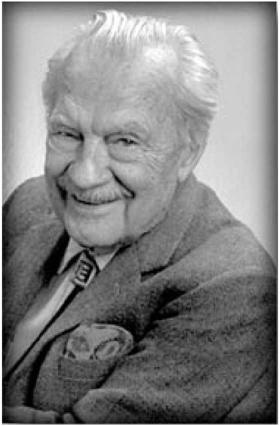
Image credit: Toni Lozano (Flickr), Yamaguchi (Wikimedia Commons)

Ulam and his solitaire

Stanislaw Ulam
1909–1984

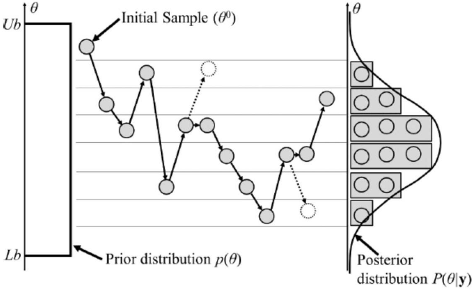
Together with Edward Teller developed the first (successful) design of the hydrogen bomb

The first thoughts and attempts I made were suggested by a question which occurred to me in 1946 as I was convalescing from an illness and playing solitaires. The question was what are the chances that a Canfield solitaire laid out with 52 cards will come out successfully? After spending a lot of time trying to estimate them by pure combinatorial calculations, I wondered whether a more practical method than "abstract thinking" might not be to lay it out say one hundred times and simply observe and count the number of successful plays.

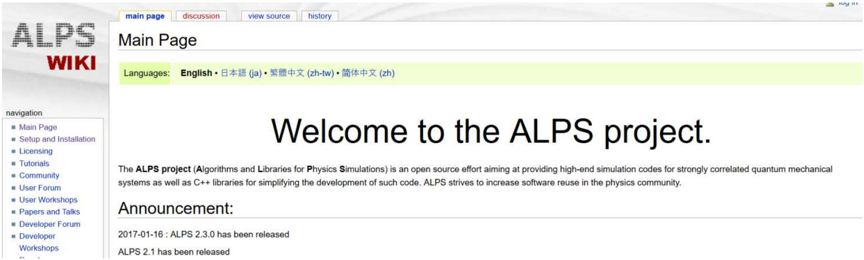


Nicholas Metropolis
1915–1999
director of the computing facility at Los Alamos

> Instead of choosing configurations randomly, then weighting them with $\exp(E/kT)$, we choose configurations with a probability $\exp(E/kT)$ and weight them evenly.
>
> N. Metropolis *et al.*
> J. Chem. Phys. 21, 1087 (1953)



J. Lee *et al.* Energies 8, 5538 (2015)



ALPS = Algorithms and Libraries for Physics Simulations
http://alps.comp-phys.org/

- Runs on different platforms (incl. Windows)
- **Diagonalization:** exact and sparse (Lanczos)
- **Monte Carlo:** classical and quantum spin models
- **Density-matrix renormalization group**
- **Dynamic mean field theory**

► Computationally not very efficient