# An introduction to Quantum Magnetism


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IPM school on spintronics and nanomagnetism

Nov. 2015

# Topics

- Lecture 1: Introduction
  - A short survey on magnetism
  - Parent Hamiltonians and exchange interaction
  - Some exotic features
- Lecture 2: Cluster operator approach
  - Spin wave theory
  - Multi-spin flip excitation (an-harmonic fluctuations)
  - Some examples

# Magnets

A permanent magnet

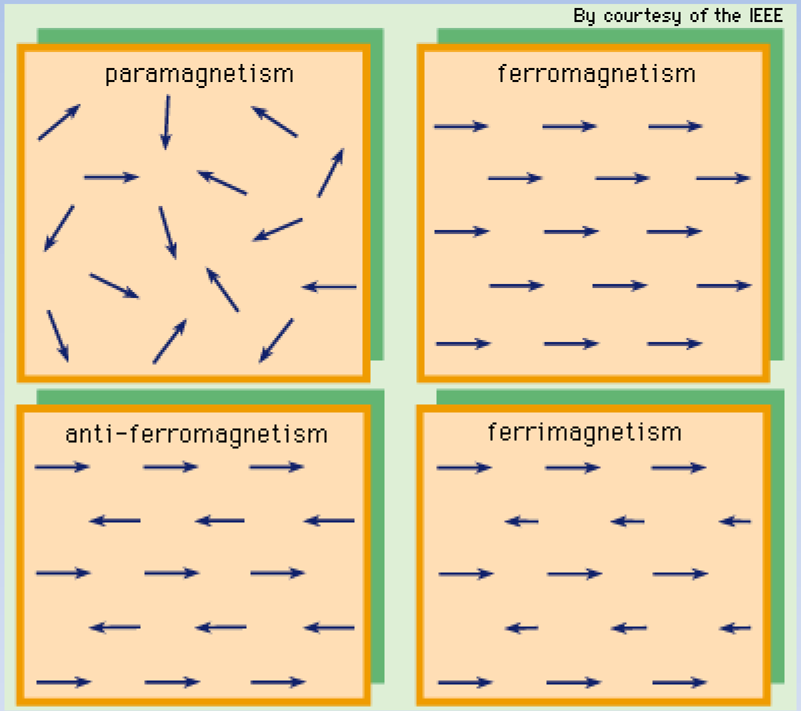
Magnetism as a result of electric current

# Different type of magnetic order: collective behavior

- Paramagnetism (response to external field),

Diamagnetism (response to external field)

- Ferromagnetism (permanent magnet)
- Antiferromagnetism (permanent magnet)
- Ferrimagnetism (permanent magnet)



# Many body systems

A system of electron and nuclei can be defined by the following Hamiltonian

$$H = H_e + H_n + H_{e-n}$$

$$H_e = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j}^{N} \frac{e^2}{|r_i - r_j|}$$

$$H_n = \sum_{i=1}^{M} \frac{P_i^2}{2M} + \sum_{i<j}^{N} \frac{(Ze)^2}{|R_i - R_j|}$$

$$H_{e-n} = -\sum_{i<j}^{N,M} \frac{Ze^2}{|r_i - R_j|}$$

Adiabatic approximation (ignoring the effect of $H_n$)

$$H \simeq H_e + H_{e-n} \equiv \sum_{i=1}^{N} (h(r_i) + V_{eff}(r_i))$$

$$h(r_i) = \sum_{i=1}^{N} \frac{p_i^2}{2m} - \sum_{i<j}^{N,M} \frac{Ze^2}{|r_i - R_j|}$$

If: kinetic energy >> potential energy

an effective potential can be found

<u>Band theory</u>

# Strongly correlated electron systems

Most of d and f orbitals have electrons with

**Potential E > Kinetic E**

Band theory fails to predict correct behavior

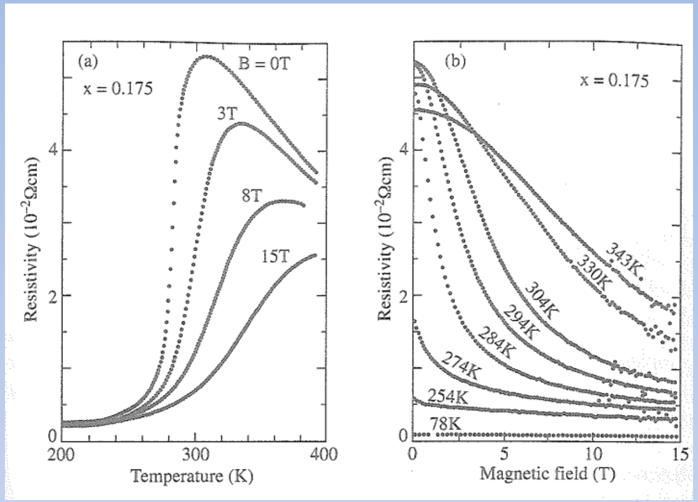



Figure 1: Colosal Magnetoresistance of $La_{1-x}Sr_xMnO_3$ for $x = 0.175$ (Tokura et.al J. Phys. Soc. Jpn.**63**, 3391 (1994). Ferromagnetic metal for $T < T_c \simeq 300$ and insulating non-magnetic property for $T > T_c$.

Example: $LaTiO_3$ (3d electrons)

It is a Mott insulator while band theory predicts to be a metal.

| Electrons | Material | Behaviour |
|---|---|---|
| 3d | $LaMnO_3$ | Colossal magnetoresistance upon doping |
| 3d | $La_2CuO_4$ | High $T_c$ superconductor upon doping |
| 4d | $Sr_2RuO_4$ | Triplet superconductor upon doping |
| ⋮ | ⋮ | ⋮ |

# Parent Hamiltonians in quantum magnetism

Consider a lattice site with four degrees of freedom

Hubbard model: $$H = t \sum_{<i,j>,\sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}) + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

For U >> t we get t-J model: $$J = \frac{4t^2}{U}, \quad n_l = \sum_\sigma n_{l,\sigma} = \sum_\sigma c^+_{l,\sigma} c_{l,\sigma}$$

$$H = \mathcal{P} \sum_{k,l} [ -t \sum_\sigma \left( c^+_{k,\sigma} c_{l,\sigma} + c^+_{l,\sigma} c_{k,\sigma} \right) + J(\mathbf{S}_k \cdot \mathbf{S}_l - \frac{1}{4} n_k n_l) ] \mathcal{P}$$

And at half-filling, we reach the Heisenberg model:

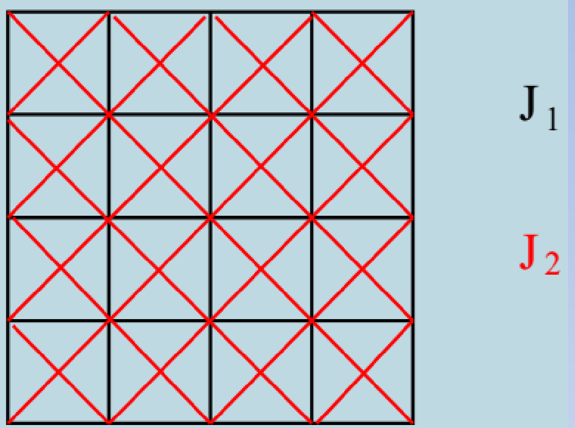
$$H = J \sum_{i,j} S_i \cdot S_j$$

# Heisenberg magnets

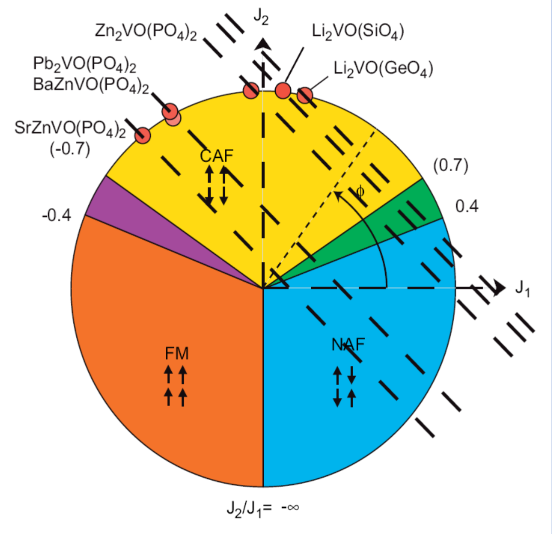
## *$J_1$-$J_2$ model*

$$H = J_1 \sum_{<i,j>} S_i \cdot S_j + J_2 \sum_{<<i,j>>} S_i \cdot S_j$$

- $Li_2VOXO_4$ where $X = Si, Ge$
- $AA'VO(PO_4)_2$ where $A, A' = Pb, Zn, Sr, Ba$




| | $q^*$ | Energy | Range $(J_1, J_2)$ | Range $\phi$ |
|---|---|---|---|---|
| NAF | $(\pi,\pi)$ | $-J_1/2 + J_2/2$ | $J_1 > 0, \quad J_2 < J_1/2$ | $-\pi/2 < \phi < \tan^{-1}(\frac{1}{2})$ |
| CAF | $(0,\pi)$ or $(\pi,0)$ | $-J_2/2$ | $\mid J_2 \mid > \mid J_1 \mid /2$ | $\tan^{-1}(\frac{1}{2}) < \phi < \pi - \tan^{-1}(\frac{1}{2})$ |
| FM | $(0,0)$ | $J_1/2 + J_2/2$ | $J_1 < 0, \quad J_2 < -J_1/2$ | $\pi - \tan^{-1}(\frac{1}{2}) < \phi < -\pi/2$ |




Classical results for different ordering,

B. schmidt et.al. J. Mag. Mag. 310, 1231 (2007)

B. Schmidt et. al. Euro. Phys. J. B. 38, 599 (2004)

# Magnetism is a pure quantum effect: Quantum Magnetism

- Bohr van Leeuwen theorem: The magnetic susceptibility will be zero for a pure classical model.

$$Q_{classic} = \int e^{-\beta H(q_i,p_i)} \prod_i d^3q_i d^3p_i$$

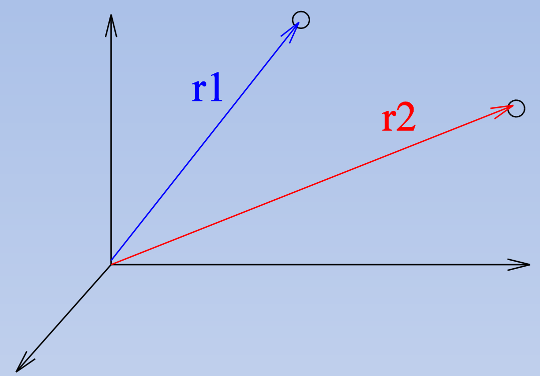
The addition of a magnetic field can be taken into account via the magnetic potential (A) via:

$$p_i \to p_i' = p_i + \frac{e}{c} A(q_i)$$

Changing the integral variables to (q_i, p'_i) with unit Jacobian gives no magnetic field dependence in the classical partition function

- The dipole-dipole interaction between magnetic moments of atoms are very small which give the critical temperature of magnetic transition some order of magnitude incorrect.

# Heisenberg interaction: Coulomb interaction + Pauli principle




Consider a system of two electrons:

$$H = h_0(r_1) + h_0(r_2) + \frac{e^2}{|r_1 - r_2|}$$

$$h_0|\phi_a> = \varepsilon_a|\phi_a>, \qquad h_0|\phi_b> = \varepsilon_b|\phi_b>, \qquad <\phi_a|\phi_b> = 0$$

The eigenstate of Hamiltonian is a Slater determinant of two orbitals:

$$|\psi_1> = \frac{1}{\sqrt{2}} det \begin{pmatrix} \phi_a(r_1)\alpha(s_1) & \phi_a(r_2)\alpha(s_2) \\ \phi_b(r_1)\alpha(s_1) & \phi_b(r_2)\alpha(s_2) \end{pmatrix}$$

$$\alpha \equiv \uparrow, \qquad \beta \equiv \downarrow$$

# Exchange interaction

There are three other Slater determinants:

$$|\psi_2 >= \frac{1}{\sqrt{2}} det \begin{pmatrix} \phi_a(r_1)\alpha(s_1) & \phi_a(r_2)\alpha(s_2) \\ \phi_b(r_1)\beta(s_1) & \phi_b(r_2)\beta(s_2) \end{pmatrix}$$

$$|\psi_3 >= \frac{1}{\sqrt{2}} det \begin{pmatrix} \phi_a(r_1)\beta(s_1) & \phi_a(r_2)\beta(s_2) \\ \phi_b(r_1)\alpha(s_1) & \phi_b(r_2)\alpha(s_2) \end{pmatrix}$$

$$|\psi_4 >= \frac{1}{\sqrt{2}} det \begin{pmatrix} \phi_a(r_1)\beta(s_1) & \phi_a(r_2)\beta(s_2) \\ \phi_b(r_1)\beta(s_1) & \phi_b(r_2)\beta(s_2) \end{pmatrix}$$

The Hamiltonian in the determinant states is:

$$H = (\varepsilon_a + \varepsilon_b)1 + \begin{pmatrix} C_{ab} - J_{ab} & 0 & 0 & 0 \\ 0 & C_{ab} & -J_{ab} & 0 \\ 0 & -J_{ab} & C_{ab} & 0 \\ 0 & 0 & 0 & C_{ab} - J_{ab} \end{pmatrix}$$

$$0 < C_{ab} = e^2 \int\int d^3r_1 d^3r_2 \frac{|\phi_a(r_1)|^2 |\phi_b(r_2)|^2}{|r_1 - r_2|}$$

$$0 < J_{ab} = e^2 \int\int d^3r_1 d^3r_2 \frac{\phi_a(r_1)^* \phi_b(r_2)^* \phi_a(r_2) \phi_b(r_1)}{|r_1 - r_2|}$$

# Effective spin Hamiltonian

$$det(H - \lambda 1) = 0 \Longrightarrow$$

$$\lambda_1 = \lambda_2 = \lambda_3 = (\varepsilon_a + \varepsilon_b) + C_{ab} - J_{ab} \equiv e_{triplet}$$
$$\lambda_4 = (\varepsilon_a + \varepsilon_b) + C_{ab} + J_{ab} \equiv e_{singlet}$$

$$e_{triplet} < e_{singlet}$$

Ferromagnetic interaction

Now consider two spin 1/2 with the following Hamiltonian:

$$H = \frac{e_{singlet} + e_{triplet}}{2} - (\frac{e_{singlet} - e_{triplet}}{2})(2S_1 \cdot S_2 + \frac{1}{2})$$

$$H_{eff} = constant - 2J_{ab}S_1 \cdot S_2$$

Question:

What happens if $< \phi_a | \phi_b > \neq 0$.

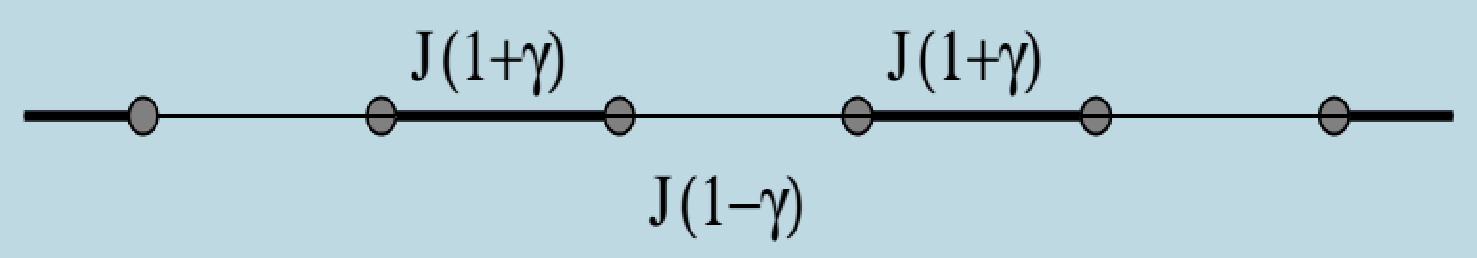
# Exotic features in spin models

➢ Haldane's conjecture (AF spin S Heisenberg chain)

$$H = J \sum_{i,j} S_i \cdot S_j$$

| $S$ | Spectrum | Correlation functions |
|---|---|---|
| Integer | Gapful | Exponential decay |
| Half integer | Gapless | Algebraic decay |

➢ Bond alternation (Affleck et.al. PRB 36 (1987) : spin-Peierls transition
Spin-1/2 bond-alternating AF chain is gapful.

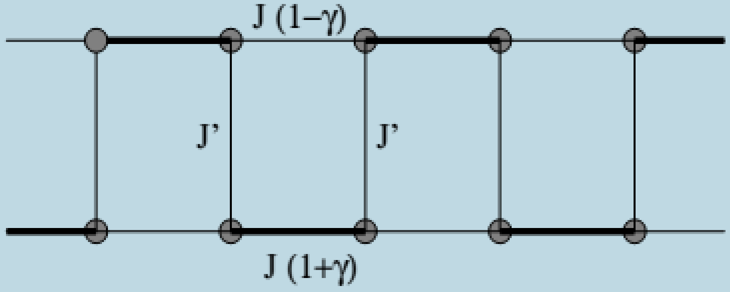


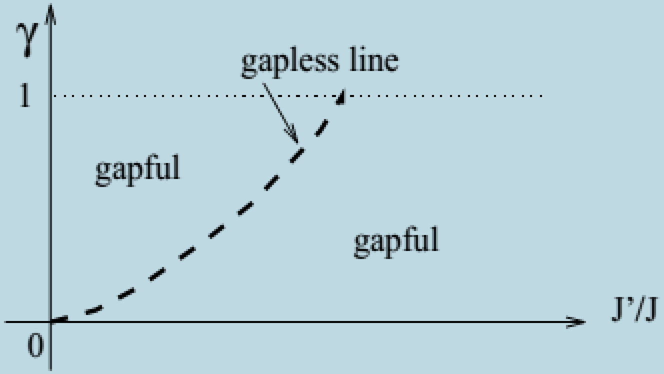
# Spin ladders (coupled chains)

- Spin-1/2 AF Heisenberg n-leg ladder

| $n$ | Spectrum | Correlation functions |
|---|---|---|
| Even | Gapful | Exponential decay |
| Odd | Gapless | Algebraic decay |

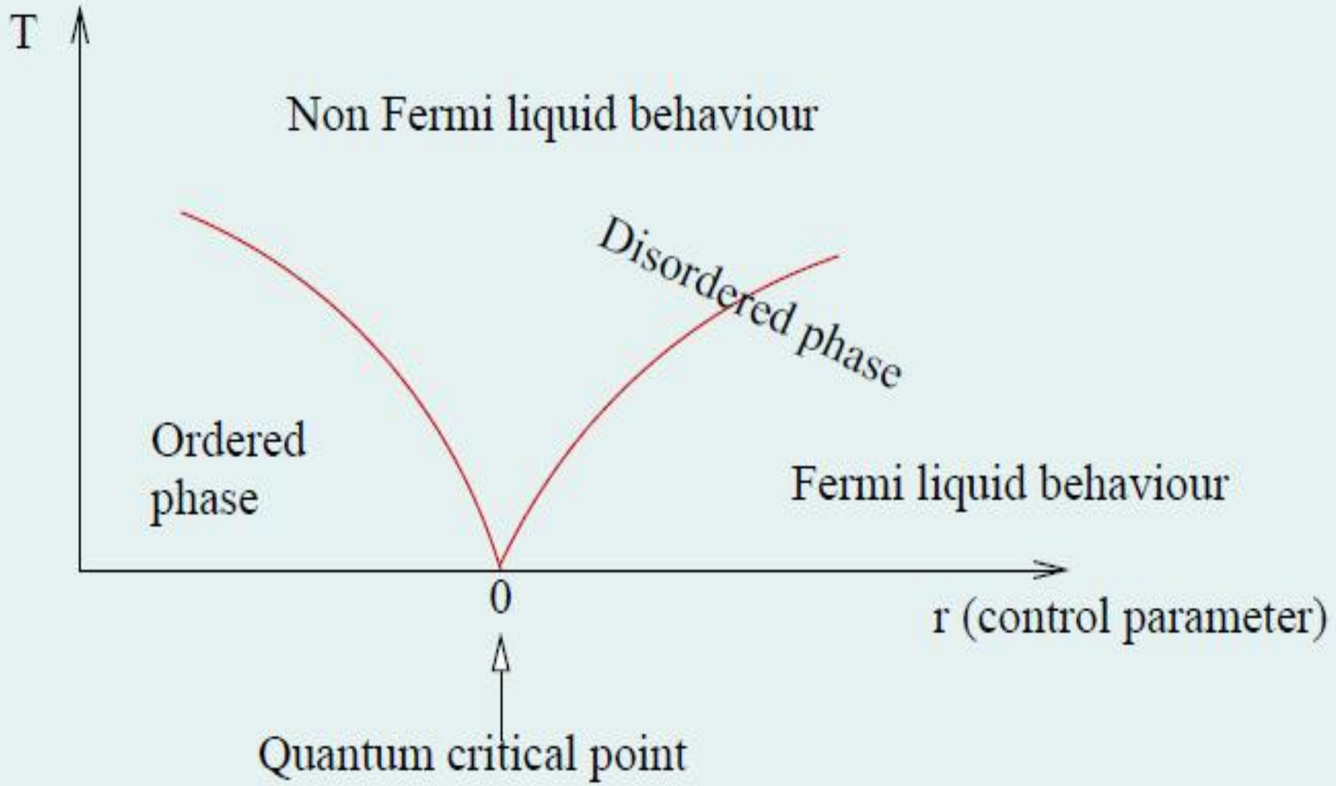
- Bond alternation (Martin-Delgado, et.al. PRL77 (1996)

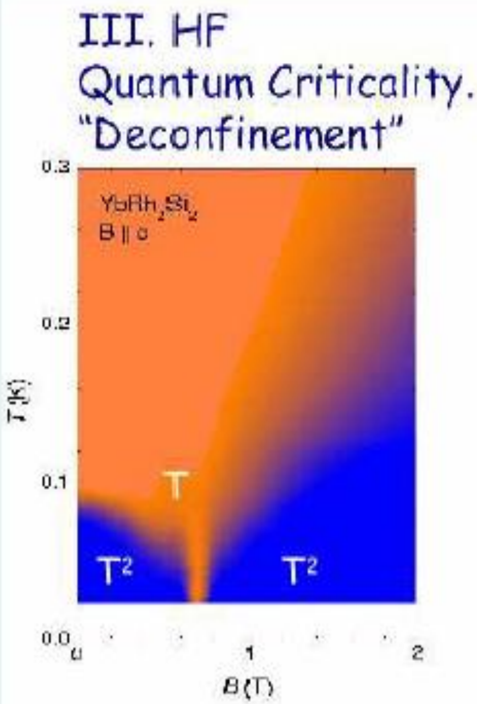


# Quantum phase transition

$$H = H_1 + r\,H_2 \quad , \quad [H_1 , H_2] \neq 0$$

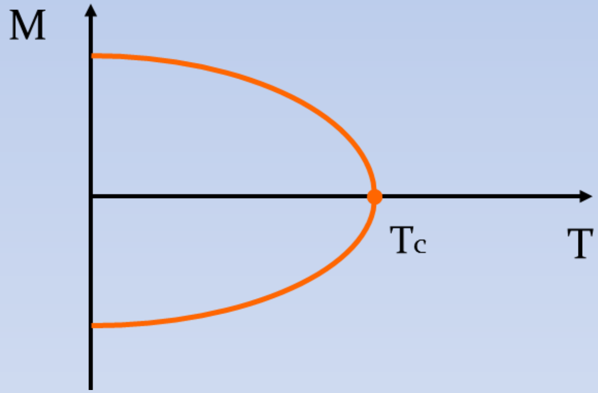


Custers et al (2004)

# Landau-Ginzburg symmetry breaking theory

- In fact particles can be organized in many different types of order, which can be explained by the Landau-Ginzburg symmetry breaking theory.
- Different order ⟺ Different symmetries




The existence of an order parameter: M

$M \neq 0$ (ordered phase)

Symmetry of the ordered phase

$G_0 = \{I\}$

$M=0$ (disorder phase)

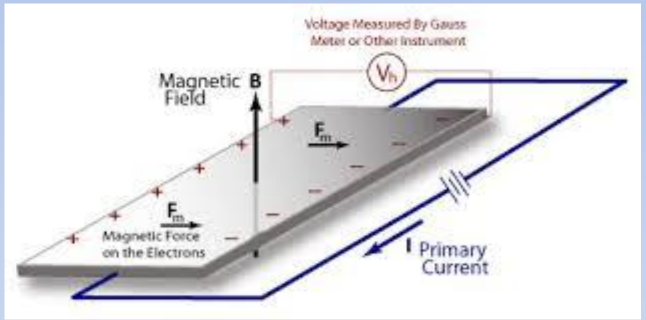
Symmetry of disorder phase

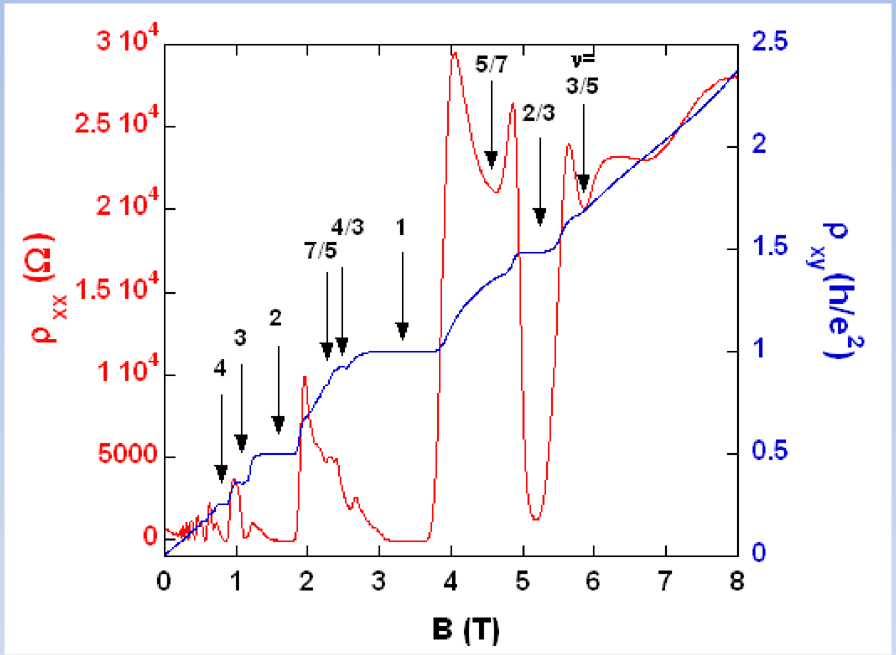
$G=\{I, \text{spin-flip}\}$

$$G_0 \subset G$$

# Does Landau paradigm explain all types of matter phases? NO!

- Fractional quantum Hall states show topological order




All states at different platueax have the same symmetry:
No symmetry breaking

(Measurements performed at NEST-SNS, Pisa)

- ❑ Other examples: spin-liquid state (a state without broken symmetry and no long-range order)

**Topological order: a new phase of matter with long-range entanglement**

# Classification of quantum phase transitions

| Landau-Ginzburg paradigm | Topological phase transition |
|---|---|
| Local order parameter | Non-local order parameter |
| Symmetry breaking | No symmetry breaking |
| Unique Ground state (or degeneracy due to symmetry) | Degenerate ground states (degeneracy due to topology) |
| Bose/Fermi quasi-particle statistics | Anyon quasi-particle statistics |
| Short-range entanglement | Long-range entanglement |

# Cluster operator approach

We will discuss in the next lecture how to find the ground state of a system to realize different phases and characterize their corresponding order.

Thanks for your attention