Statistical Field Theory Lattice models

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Lattices (1)

Bar of ferromagnetic metal, embedded in a magnetic field B: statistical system of atoms ordered in a metallic lattice Λ

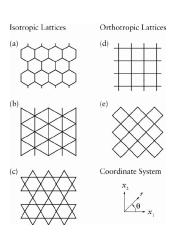
Sites described by vectors $n \in \Lambda$, linear combinations of a base $\{e_{\mu}; \mu = 1, ..., D\}$ in \mathbb{R}^{D} , not necessarily orthonormal, with integer coefficients $n_{\mu} \in \mathbb{Z}$

$$n=\sum_{\mu=1}^D n_\mu e_\mu$$

 e_{μ} need not to be orthogonal. Vectors f^{μ} such that

$$f^{\mu}\cdot e_{
u}=\delta^{\mu}_{
u}$$

are a basis in the dual lattice Λ^* .



Lattices (2)

Summation on sites of the lattice

$$\sum_{\langle n,m\rangle} s_n s_m$$

Notation $\langle n, m \rangle$ means m is nearest neighbour to n in the lattice Λ

▶ It contains $\zeta N/2$ terms, where $\zeta =$ number of nerarest neighbous of a site, is called *coordination number* of the lattice

$$\zeta = \begin{cases} 2 & \text{in } D = 1 \text{ (spin chain)} \\ 4 & \text{in } D = 2 \text{ on a square lattice} \\ 3 & \text{in } D = 2 \text{ on a hexagonal lattice} \\ 6 & \text{in } D = 3 \text{ on a cubic lattice} \\ & \text{etc...} \end{cases}$$

➤ Sites are connected by links (or bonds). The most elementary closed paths of links are called faces (or tiles, or plaquettes)

Ising model

- Ferromagnetism: in a metal, atomic spins (magnetic moments) all point in the same direction, yielding a net magnetic moment, macroscopic in size.
 - Atoms thought as magnetic dipoles (spin). Align in presence of an external magnetic field.
 - Magnetic dipoles interact also with each other



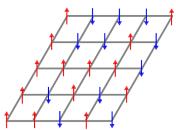
Ising model: (E. Ising & W. Lenz) Simplest classical theoretical description of ferromagnetism. Variables s_n take values ± 1 .

$$H[s_n] = -J\sum_{\langle n,m\rangle} s_n s_m - B\sum_n s_n$$

Statistical system conveniently described in function of the two independent thermodynamical variables: temperature \mathcal{T} , external magnetic field \mathcal{B}



Physics of the Ising model (1)



First term in the hamiltonian

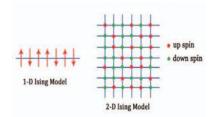
$$-J\sum_{n,\mu}s_ns_m$$

overall energy is lowered when neighbouring atomic spins are aligned.

Due to the Pauli exclusion principle: two electrons on neighbouring atoms with parallel spins cannot come close together in space. No such restriction applies if the electrons have anti-parallel spins.

Physics of the Ising model (2)

- ▶ Different spatial separations imply different electrostatic interaction energies. Exchange (electrostatic) energy J measures this difference. It can be quite large: i.e., $J \sim 1 \text{eV}$.
- ▶ Energy associated with the direct magnetic interaction between neighbouring atomic spins $\sim 10^{-4} \text{eV}$.
- ► However, the exchange effect is very short-range ⇒ restriction to nearest neighbour interaction is quite realistic.



Ising model

Partition function

$$Z(T,B) = \sum_{\{s_n\}} e^{-\beta H[s_n]}$$

where $\{s_n\}$ represents a configuration of the spins s_n on all the sites n of the lattice. The sum has to be performed on all the possible configurations. The phase diagram consists in a plane (T,B). The free energy

$$F(T,B) = -k_B T \log Z(T,B) = -\frac{1}{\beta} \log Z(\beta,B)$$

is the generating functional of all the physical observables of the system. As it is an extensive quantity proportional to the number of sites N, it is often convenient (thinking to the thermodynamic limit $N \to \infty$) to consider the free energy per site

$$\mathcal{F}(T,B) = \frac{1}{N}F(T,B) = -\frac{1}{N\beta}\log Z(\beta,B)$$

Magnetization

$$M(\beta, B) = \frac{\partial F}{\partial B} = -\frac{1}{\beta Z} \frac{\partial Z}{\partial B} = -\frac{1}{\beta Z} \sum_{\{s_n\}} \frac{\partial}{\partial B} e^{-\beta H[s_n]}$$
$$= \frac{1}{Z} \sum_{\{s_n\}} \left(\sum_{n} s_n \right) e^{-\beta H[s_n]} = \langle \sum_{n} s_n \rangle = \sum_{n} \langle s_n \rangle$$

If the system is translation invariant, which is true for an infinite lattice or for a finite lattice with periodic boundary conditions we have

$$\langle s_n \rangle = \langle s_0 \rangle$$
 , $\forall n \in \Lambda$

0 is a point of the lattice origin of the reference frame.

$$M = N\langle s_0 \rangle$$

It is an extensive quantity. Convenient to introduce the magnetization per site

$$\mathcal{M} = \frac{M}{N} = \langle s_0 \rangle$$

Other physical quantities

magnetic susceptivity per site at constant temperature

$$\chi = \left. \frac{\partial \mathcal{M}}{\partial B} \right|_{B=0} = N \left. \frac{\partial^2 F}{\partial B^2} \right|_{B=0} = \frac{1}{Nk_B T} \sum_n \left(\langle s_n s_0 \rangle - \langle s_0 \rangle^2 \right)$$

internal energy

$$U = F - T \frac{\partial F}{\partial T}$$

thermal capacity (or specific heath)

$$C = T^2 \frac{\partial^2 F}{\partial T^2}$$

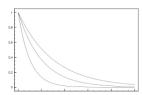
Correlation functions

- Measure of conditional probability that the value of the spin variable at a point may influence the values on other lattice sites
- ► The 2 point function

$$G^{(2)}(i,j) \stackrel{\mathrm{def}}{=} \langle s_i s_j \rangle = \frac{1}{Z} \sum_{\{s_i\}} s_i s_j e^{-\beta H[s_i]}$$

measure of relative alignement of spins i and j.

In a translationally invariant system $G^{(2)}$ depends only the difference i-j. If also rotationally invariant on distances $r\gg a$, where a is the lattice spacing, it depends only on distance r=|i-j|.



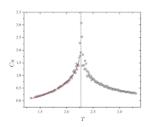
Correlation length

▶ Ferromagnetic phase $\mathcal{M} \neq 0$: it is convenient to define a connected 2 point function

$$G_c^{(2)}(r) = \langle (s_i - s_0)(s_j - s_0) \rangle = \langle s_i s_j \rangle - \langle s_0 \rangle^2$$

- ▶ Paramegnetic phase $\mathcal{M} = 0$: the two definitions coincide.
- Near neighbour spins tend to align but as the distance increases the correlation becomes weaker. Normally, an exponential decrease is observed, with a characteristic length, the correlation length ξ

$$G_c^{(2)}(r) \simeq e^{-\frac{r}{\xi}}$$
 for $r \gg a$ and $T \neq T_c$



Correlation function at criticality

At the critical point $\xi \to \infty$ and all the spins tend to be correlated. Collective phenomena arise at large scale.

Correlation function decays as a power law

$$G_c^{(2)}(r)\simeq \frac{1}{r^{D-2+\eta}}$$

 η is a critical exponent called anomalous dimension. Correlation length diverges at the critical point with a power law

$$\xi(T) \underset{t \to 0^{\pm}}{\sim} \xi_{\pm} |t|^{-\nu_{\pm}}$$

thus defining another critical exponent u