Magnetism. 3: Mean-Field Ferromagnetism

General Considerations

• *Idea:* Ferromagnetic materials are an example of system in which each atom has a permanent magnetic dipole moment $\vec{\mu}$, related to its spin by $\vec{\mu} = g\mu_0\vec{s}$, where $\mu_0 = e\hbar/2mc$ is the Bohr magneton and g a dimensionless number of order unity (the Landé g-factor). Contrary to what happens in paramagnetic materials, however, electrons in neighboring atoms interact with each other, mostly through an *electrostatic* exchange interaction. In a ferromagnet therefore even classically $Z_N \neq Z_1^N/N!$, and thermal fluctuations have to compete not just with the possible aligning effect of an external magnetic field, but with the intrinsic aligning effect of the interactions as well. We will assume that the atoms are located at fixed lattice sites i.

• *Hamiltonian:* Since we neglect translational motion, the effective degrees of freedom are simply the values of the spins $\vec{s}_i$ at all lattice sites. The exchange interaction between the electrons can be effectively described by a symmetric matrix J^{ij}, so their total Hamiltonian in an external magnetic field $\vec{B}_{\rm ext} = B\,\hat{\mathbf{z}}$ is

$$H = -\sum\nolimits_{i,\,j\neq i} J^{ij}\,\vec{s}_i\cdot\vec{s}_j - \sum\nolimits_i \vec{\mu}_i\cdot\vec{B}_{{\rm ext},i}\ .$$

We now notice that each $\vec{s}_i$ sees an effective magnetic field due to both $\vec{B}_{{\rm ext},i}$ and the effect of all other spins,

$$H = -g\mu_0\sum\nolimits_i \vec{B}_{{\rm eff},i}\cdot\vec{s}_i\ ,\qquad \text{with}\qquad \vec{B}_{{\rm eff},i} := \vec{B}_{{\rm ext},i} + (g\mu_0)^{-1}\sum\nolimits_{j\neq i} J^{ij}\,\vec{s}_j\ .$$

• *Weiss mean-field theory:* Although in principle any two spins in the lattice interact with each other and each $\vec{s}_i$ feels the actual value of all other spins, in this theory we start by approximating the situation by an interaction of $\vec{s}_i$ with the mean value of each of the other spins, and use as Hamiltonian

$$H' = -g\mu_0\sum\nolimits_i \langle\vec{B}_{{\rm eff},i}\rangle\cdot\vec{s}_i\ ,\qquad \text{with}\qquad \langle\vec{B}_{{\rm eff},i}\rangle = \vec{B}_{{\rm ext},i} + (g\mu_0)^{-1}\sum\nolimits_{j\neq i} J^{ij}\,\langle\vec{s}_j\rangle\ .$$

Notice that this ignores correlations, which actually changes the physical problem. Neglecting boundary effects, if the system (the lattice and the J^{ij}) has symmetries under translations and rotations around the z axis, in the mean-field approach the effective magnetic field will be parallel (or antiparallel) to $\vec{B}_{\rm ext}$ and its z component $\langle B_{{\rm eff},i}\rangle = B + (g\mu_0)^{-1}\sum_{j\neq i} J^{ij}\,\langle s_{j,z}\rangle$. The set of solutions for the $\{\vec{s}_i\}$ will then have the same symmetries, though this does not imply that in one solution all $\vec{s}_i$ do, or have the same value.

Mean Magnetization

• *Goal:* Choose again coordinates such that $\langle\vec{B}_{{\rm eff},i}\rangle = \langle B_{{\rm eff},i}\rangle\,\hat{\mathbf{z}}$. We want to find $\bar{M} = \sum_i\langle\mu_i\rangle = g\mu_0\sum_i\langle s_i\rangle$.

• *Setup:* We will treat the system quantum mechanically. We could calculate $F = -k_{\rm B}T\ln Z$ and $\bar{M} = -\partial F/\partial B|_T$, or use the density matrix and find the mean value of the spin directly as $\langle s_i\rangle = {\rm tr}(\hat\rho\,\hat{s}_i)$. In our approximation $\hat{H}'$ is a sum of terms from individual spins so, since the eigenvalues of $\hat{s}_i = \hat{s}_{i,z}$ are $s_i = \pm\,\frac12\hbar$,

$$\begin{aligned}\langle s_i\rangle &= \frac{{\rm tr}\,\hat{s}_i\,{\rm e}^{-\beta\hat{H}'}}{{\rm tr}\,{\rm e}^{-\beta\hat{H}'}} = \frac{\sum_{s_i} s_i\,{\rm e}^{\beta g\mu_0\langle B_{{\rm eff},i}\rangle s_i}}{\sum_{s_i}{\rm e}^{\beta g\mu_0\langle B_{{\rm eff},i}\rangle s_i}}\\ &= \frac{\hbar}{2}\tanh\left(\tfrac12\,\beta g\mu_0\hbar\,\langle B_{{\rm eff},i}\rangle\right) = \frac{\hbar}{2}\tanh\left\{\tfrac12\,\beta\hbar\left(g\mu_0 B + \textstyle\sum_{j\neq i}J^{ij}\langle s_j\rangle\right)\right\}\ .\end{aligned}$$

If all the $\langle s_i\rangle$ are the same (note–this is not true in antiferromagnetic materials), we can denote their value simply by $\langle s\rangle$. We then introduce the quantities $\tilde{J} := \sum_{j\neq i}J^{ij}$ (for example, if $J^{ij} = J$ when i and j are nearest neighbors and 0 otherwise, then $\tilde{J} = \nu J$, where ν is the number of nearest neighbors of each lattice site), $x := \frac12\,\beta\hbar\tilde{J}\langle s\rangle$ and $b := \frac12\,\beta\hbar g\mu_0 B$,

$$\langle s\rangle = \frac{\hbar}{2}\tanh\left\{\tfrac12\,\beta\hbar\,(\tilde{J}\langle s\rangle + g\mu_0 B)\right\}\ ,\qquad \text{or}\qquad \frac{4}{\beta\hbar^2\tilde{J}}\,x = \tanh(x+b).$$

The most interesting case is $\vec{B}_{\rm ext} = 0$, which leads to a spontaneous magnetization $\bar{M} = N\langle\mu_z\rangle = Ng\mu_0\langle s_z\rangle$.

• *Graphical solution:* For a fixed value of β, the solutions for $\langle s\rangle$ correspond to the values of x where the straight line $(4/\beta\hbar^2\tilde{J})\,x$ and the curve $\tanh(x+b)$ intersect. [∗ see the plot ∗]

• *Phase transition:* When $B = 0$ (or $b = 0$), the solutions are qualitatively different for T above and below the critical Curie temperature,

$$T_{\rm c} = \frac{\hbar^2\tilde{J}}{4k_{\rm B}}\ .$$

High temperature: For $4/\beta\hbar^2\tilde{J} \geq 1$, or $T > T_{\rm c}$, there is 1 solution, $x = 0$ (paramagnetism).
Low temperature: For $4/\beta\hbar^2\tilde{J} < 1$, or $T < T_{\rm c}$, there are three solutions, $x = 0$ and $x_\pm$, the two new ones corresponding to spontaneous magnetization. To determine which solutions actually occur and are physical, we study the susceptibility χ, below. (Another approach would be to use general thermodynamical considerations on phase transitions and stability.)

• *Remark:* When $\vec{B}_{\rm ext} = 0$, only the *set* of solutions must be symmetric about $\langle s\rangle = 0$, but an individual solution can have either $\langle s\rangle > 0$ or $\langle s\rangle < 0$. This is an example of spontaneous breaking of symmetry.

Susceptibility

• *Calculation:* To calculate $\chi \propto \partial\langle s\rangle/\partial B$ for a single atom, we need to reintroduce an external magnetic field $\vec{B}_{\rm ext} = B\,\hat{\mathbf{z}}$. Then from the implicit expression above for $\langle s\rangle$ above we get

$$\langle s\rangle = \frac{\hbar}{2}\tanh\left(\tfrac12\,\beta\hbar\,(\tilde{J}\langle s\rangle + g\mu_0 B)\right)\ ,\qquad \text{and}\qquad \chi := \frac{\partial\langle s\rangle}{\partial B} = \frac{\hbar}{4}\,\frac{\beta\hbar\,(\tilde{J}\chi + g\mu_0)}{\cosh^2\left(\tfrac12\,\beta\hbar\,(\tilde{J}\langle s\rangle + g\mu_0 B)\right)}\ .$$

(To simplify the plot for a graphical solution, in this case we can define $x := \frac12\,\beta\hbar\,(\tilde{J}\langle s\rangle + g\mu_0 B)$.)

• *Physical value of $\langle s\rangle$ for $B = 0$:* Setting $B = 0$ and $\langle s\rangle = 0$ in the last equation and simplifying, we find that the zero-field susceptibility is

$$\chi(T) = \frac{1}{4k_{\rm B}}\,\frac{1}{T - T_{\rm c}}\ ,\qquad T_{\rm c} = \frac{\hbar^2\tilde{J}}{4k_{\rm B}}\ .$$

Thus, for $T < T_{\rm c}$ the susceptibility χ would be negative, which signals an unstable state and indicates that $\langle s\rangle = 0$ is not a physical solution.

• *Phase transition:* As T approaches $T_{\rm c}$, the $(T - T_{\rm c})^{-1}$ behavior of χ denotes a second-order phase transition with order parameter T and critical exponent -1 (associated with a SO(3) $\mapsto$ SO(2) phase transition).

⋆ *Remark:* One can also see the phase transition by calculating the mean energy $\bar{E}(T)$ and the heat capacity $C = \partial\bar{E}/\partial T$ for $B = 0$.

Improved Models

• *Idea:* The Weiss mean-field theory of ferromagnetism predicts the existence of a phase transition in every dimensionality. More detailed models, such as the Ising model and the Heisenberg models, make qualitatively different predictions, including the absence of a phase transition in one dimension. Some of these models can be exactly solved, others need to be treated with other approximation methods or numerically.

Reading

• *Course textbook:* Kennett, § 10.2.
• *Other books:* Pathria & Beale, Chapter 12, especially § 12.5; Chandler, § 5.4–5.5 (pp 131–138); Plischke & Bergersen, mentioned in § 1.8; Reif, §§ 10.6–10.7, including a clear physical explanation of the exchange interaction; Schwabl, §§ 6.6 and 7.1.2.