

A 3 Localized Moments: Finite Temperature

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1 Introduction

Ferromagnetic materials are important constituents of many modern hi-tech devices. Interestingly, the most important property of a ferromagnetic system, its spontaneous magnetization (without applying an external magnetic field) is temperature dependent. Since for technological applications magnetic devices must have operating temperatures of about room temperature or even higher the understanding of the influence of temperature on magnetic systems is an important part of today's research.

A ferromagnetic system has a critical temperature, the so-called Curie temperature T_c , above which the spontaneous magnetization remains zero while it is finite below T_c . The disappearance of the spontaneous magnetization is an example for a phase transition of second order where the spontaneous magnetization is the order parameter characterizing the phase transition, vanishing continuously at T_c . For second order phase transitions an important principle exists, namely *universality*. Universality means that the behavior of a system close to its critical point does not depend on details of the system such as its material parameters or the geometry of the sample. Instead, physical systems fall into so-called *universality classes* depending only on symmetry of the underlying model such as the spatial dimension of the system, or — in a magnetic system — the dimension of the spins.

From the theoreticians point of view one interesting point about nano-technology is that the size of a physical system is reduced almost to an atomic level so that one can prepare and investigate samples like very thin films where the crossover from three to two dimensional behavior can be studied and even chains of atoms which behave effectively one dimensional. For systems of small spatial extension thermal activation is an important issue since smaller systems often also have smaller energy barriers separating different states of the system which then could be overcome by thermal activation. Many interesting questions have to be explored, like, e. g., what is when a system is of nanometer size in one, two, or even in all three dimensions? Is a spin chain or a nano-particle still a ferromagnet?

The following lecture will focus on the temperature dependence of the spontaneous magnetization, on the calculation of the critical temperature and on the question under which conditions magnetic order exists, especially when reducing the dimension of the system from three to lower dimension. We will do this within the framework of models of localized magnetic moments, using the Heisenberg model. Since exact analytical solutions can hardly be obtained we have to use approximations. We start with the mean-field theory where a first, simple description of the ferromagnetic phase transition can be obtained. We will discuss the classical limit and compare the mean-field results with Monte Carlo simulations. For a deeper understanding of magnetic order in lower dimensions we need better approximation and as an example we will have an introduction to the theory of Tjabykov. This theory provides a better estimate of the critical temperature and it gives a first idea that magnetic order cannot occur in a one or two dimensional isotropic Heisenberg model. This is the contents of the *Mermin-Wagner theorem* and we will see that in two dimensions magnetic order can occur only in systems with a magnetic anisotropy so that the system falls into the Ising universality class while there is no thermally stable ferromagnetic order in one dimension.

2 Mean-Field approximation for the Heisenberg model

Throughout this lecture we will describe a magnetic system using a model of spins which are localized on a given lattice, a quantum mechanical Heisenberg model [1] (see Refs. [2, 3, 4] for a review of the theoretical background). In general the Hamiltonian of a spin model describing a magnetic system may contain contributions from exchange energy, crystalline anisotropies, a coupling of the magnetic moments of the spins to an external magnetic field (Zeeman energy), and from the dipole-dipole interaction of the spins (magneto-static energy) — among others — where the latter is the microscopic origin of the stray field energy and the shape anisotropy. Since the exchange energy and the Zeeman energy are usually the largest contributions and, hence, most important for a first understanding of the ferromagnetic phase transition we neglect the others for the moment and start with the Hamiltonian

$$\mathcal{H} = -\frac{J}{2\hbar^2 S^2} \sum_{i,j} \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j - \frac{g\mu_B B}{\hbar} \sum_i \tilde{S}_i^z. \quad (1)$$

The z -axis of our coordinate system is aligned with the magnetic field B . g is the Landé factor and μ_B is Bohr's magneton. We assume that the spins are located on a regular lattice neglecting any kinds of disorder or boundary effects. Furthermore let us assume in this chapter that there is only nearest neighbor exchange interaction. Then there is only one exchange coupling constant J and for $J > 0$ the Hamiltonian favors ferromagnetic order, i. e., parallel alignment of the spins $\tilde{\mathbf{S}}_i$. The factor 2 in the denominator of the first term comes from the fact that each interaction is counted twice in the double sum. S is the spin quantum number and the factor $\hbar^2 S^2$ is a normalization of the spin product to its largest eigenvalue so that J is an exchange energy constant describing the energy difference between parallel and antiparallel states of two spins. As usual we can introduce the creation and destruction operators $\tilde{S}_i^\pm = \tilde{S}_i^x \pm i\tilde{S}_i^y$ so that the Hamiltonian can be rewritten in the form

$$\mathcal{H} = -\frac{J}{2\hbar^2 S^2} \sum_{i,j} \left(\tilde{S}_i^+ \tilde{S}_j^- + \tilde{S}_i^- \tilde{S}_j^+ \right) - \frac{g\mu_B B}{\hbar} \sum_i \tilde{S}_i^z. \quad (2)$$

In the ground state ψ_0 of the system all spins are parallel (and in z direction aligned with the field) and with $\tilde{S}_i^+ \psi_0 = 0$ and $\tilde{S}_i^z \psi_0 = \hbar S \psi_0$ we get for the ground state of the system the energy $E = -JzN/2 - g\mu_B BSN$ and the magnetic moment $\mathbf{M} = N\hbar S e_z$ where z is the number of nearest neighbors in the lattice structure under consideration and N the number of spins.

In order to understand the temperature dependence of the reduced magnetization $\mathbf{m}(T)$ we have to calculate

$$\mathbf{m}(T) = \frac{\mathbf{M}(T)}{M(0)} = \frac{1}{\hbar SN} \sum_i \langle \tilde{\mathbf{S}}_i \rangle = \frac{1}{\hbar SN} \text{Tr} \frac{1}{Z} e^{-\mathcal{H}/k_B T} \sum_i \tilde{\mathbf{S}}_i \quad (3)$$

where $\langle \dots \rangle$ denotes a thermal average and $Z = \text{Tr} e^{-\mathcal{H}/k_B T}$ is the canonical partition function. The expression above cannot be calculated exactly. Instead we have to use approximations and the simplest approximation is the mean-field approximation [5, 6, 7].

With $\tilde{\mathbf{S}}_i = (\tilde{\mathbf{S}}_i - \langle \tilde{\mathbf{S}}_i \rangle) + \langle \tilde{\mathbf{S}}_i \rangle$ the operator product in our Hamiltonian becomes

$$\tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j = (\tilde{\mathbf{S}}_i - \langle \tilde{\mathbf{S}}_i \rangle) \cdot (\tilde{\mathbf{S}}_j - \langle \tilde{\mathbf{S}}_j \rangle) + (\tilde{\mathbf{S}}_i - \langle \tilde{\mathbf{S}}_i \rangle) \cdot \langle \tilde{\mathbf{S}}_j \rangle + \langle \tilde{\mathbf{S}}_i \rangle \cdot (\tilde{\mathbf{S}}_j - \langle \tilde{\mathbf{S}}_j \rangle) + \langle \tilde{\mathbf{S}}_i \rangle \cdot \langle \tilde{\mathbf{S}}_j \rangle$$

and the idea behind mean-field approximation is to neglect the first part of the sum which is the correlation of deviations from the thermal average at lattice sites i and j . With this simplification our mean-field Hamiltonian becomes

$$\begin{aligned}\mathcal{H}_{\text{MF}} &= -\frac{J}{\hbar^2 S^2} \sum_{i,j} \tilde{\mathbf{S}}_i \cdot \langle \tilde{\mathbf{S}}_j \rangle + \frac{J}{2\hbar^2 S^2} \sum_{i,j} \langle \tilde{\mathbf{S}}_i \rangle \cdot \langle \tilde{\mathbf{S}}_j \rangle - \frac{g\mu_B B}{\hbar} \sum_i \tilde{S}_i^z \\ &= -\frac{Jzm + g\mu_B BS}{\hbar S} \sum_i \tilde{S}_i^z + \frac{J}{2} Nz m^2,\end{aligned}\quad (4)$$

where m is the z component of the magnetization vector \mathbf{m} . For the second part of the equation above we have assumed that the magnetization is in z direction and that $\langle \tilde{\mathbf{S}}_i \rangle$ is identical everywhere in the lattice. Formally, this is now the same problem as that of spins which are interacting only with a field (paramagnetic spins, see e. g. [8]). The only difference is that the so-called molecular field here consists of an external field plus an exchange field which is represented by the magnetization of the z neighbors. The reduced magnetization can now be calculated as

$$m(T) = \frac{\langle \tilde{S}_i^z \rangle}{\hbar S} = \frac{\text{Tr} \tilde{S}_i^z e^{-\mathcal{H}_{\text{MF}}/k_B T}}{\hbar S \text{Tr} e^{-\mathcal{H}_{\text{MF}}/k_B T}} = \frac{\text{Tr} \tilde{S}_i^z e^{(Jzm + g\mu_B BS)\tilde{S}_i^z/\hbar S k_B T}}{\hbar S \text{Tr} e^{(Jzm + g\mu_B BS)\tilde{S}_i^z/\hbar S k_B T}}.$$

Within the mean-field approximation we are left with an effective single-spin problem and the trace is now simply a sum over all quantum numbers $\sum_{l=-S}^S$ so that

$$\begin{aligned}m(T) &= \frac{\sum_{l=-S}^S l e^{(Jzm + g\mu_B BS)l/S k_B T}}{S \sum_{l=-S}^S e^{(Jzm + g\mu_B BS)l/S k_B T}} \\ &= \frac{2S + 1}{2S} \coth \frac{(2S + 1)(Jzm + g\mu_B BS)}{2S k_B T} - \frac{1}{2S} \coth \frac{(Jzm + g\mu_B BS)}{2S k_B T} \\ &= B_S \left((Jzm + g\mu_B BS)/k_B T \right).\end{aligned}\quad (5)$$

Here, $B_S(x)$ is called Brillouin function which is defined in the line above. For the special case $S = 1/2$ the Brillouin function is simply

$$B_{1/2}(x) = \tanh(x).$$

However, in both cases Eq. 5 is a so-called self consistency equation where the unknown variable $m(T)$ is on both sides of the equation such that one cannot find an analytical solution. But one can find numerical solutions easily: subtracting $m(T)$ on both sides of the equation we are left with a root finding problem for which numerical algorithms exist [9].

Fig. 1 shows $m(T)$ data for $B = 0$ and different quantum numbers obtained from a numerical solution of Eq. 5 for $z = 6$ corresponding to a simple cubic lattice. The magnetization decreases with increasing temperature and vanishes at a critical temperature T_c which depends on the quantum number. A self consistency equation can have more than one solution. In our case $m(T) = 0$ is always a possible solution but below T_c there exists also a solution with finite $m(T)$ and, furthermore, apart from the solution shown in Fig. 1 there exists also a solution with a negative m and the same absolute value. However, one can prove by calculating the free energy that the solutions with $m \neq 0$ have a lower free energy corresponding to the thermally

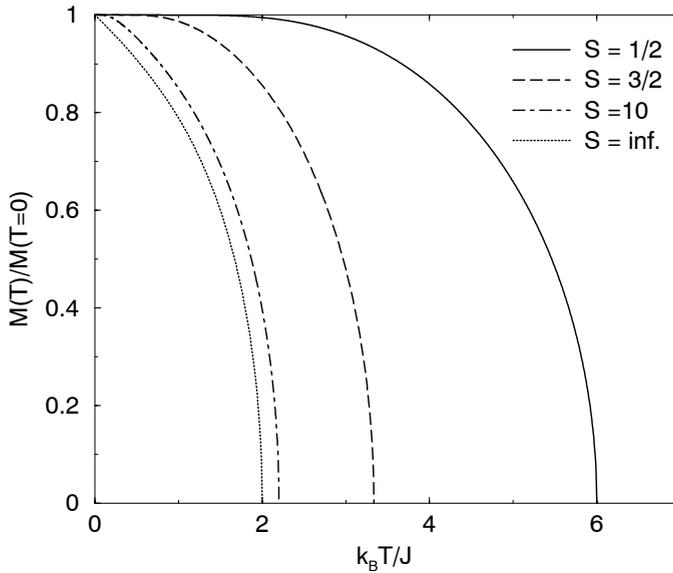


Fig. 1: Numerical solution of the mean-field self consistency equation (Eq. 5) for a number of nearest neighbors $z = 6$ as in a simple cubic lattice [10]. Shown is the temperature dependence of the magnetization for $B = 0$ and different quantum numbers.

stable state. Numerically, it depends on the initial state one starts the calculation with which of the different solutions of the self-consistency equation one will obtain.

Since in the critical region — close to T_c — $m(t)$ is small the Brillouin function can be expanded,

$$B_S(x) = \frac{S(S+1)}{3S}x - \frac{(S+1)(2S^2+2S+1)}{90S^3}x^3 + \mathcal{O}(x^5)$$

From the first term T_c can be calculated,

$$k_B T_c = \frac{zJ(S+1)}{3S}. \quad (6)$$

Note that in the mean-field approximation T_c is simply proportional to the number of neighbors and does not depend on the dimension of the system or its lattice structure. We will show later that this is not realistic.

From the next term in the expansion above the behavior of the magnetization close to T_c can be calculated leading to

$$m(T \rightarrow T_c) \sim (T_c - T)^\beta \quad \text{for } T < T_c \quad (7)$$

with $\beta = 1/2$. Power laws are typical for phase transitions of second order [11, 12] and in the case of a ferromagnetic phase transition the spontaneous magnetization is the order parameter which characterizes the transition (it is zero above and finite below the transition). Second order means that the order parameter vanishes continuously while for a phase transition of first order the order parameter would jump at T_c . β is called the critical exponent of the order parameter.

For small but finite magnetic field B the same expansion can be used to calculate the susceptibility in the paramagnetic regime,

$$\chi(T \rightarrow T_c) \sim |T - T_c|^{-\gamma} \quad (8)$$

where $\gamma = 1$ is another critical exponent. This is the well known Curie-Weiss law.

For second order phase transitions an important principle exists, namely *universality* [11, 12]. Universality means that the behavior of a system (characterized by its critical exponents) close to its critical point (here $B = 0$, $T = T_c$) is universal in the sense that it does not depend on details of the system such as its material parameters or the lattice structure. Instead, physical systems fall into so-called *universality classes* depending only on symmetry of the underlying model such as the spatial dimension of the system, or — in a magnetic system — the dimension of the spins. Nevertheless, even for models belonging to the same universality class the value of T_c might well depend on all the details of the Hamiltonian.

While the mean-field approach gives a nice qualitative description of phase transitions, quantitatively it is less correct. In reality T_c does not depend on the number of neighbors only, instead it depends also on the lattice structure and especially on the dimension of the lattice. Indeed we will see later on that eventually there is no ferromagnetic transition in two and one dimensional systems at all. Furthermore, the critical exponents which we calculated before (we had $\beta = 1/2$ and $\gamma = 1$ but there are also other related exponents coming e. g. from the specific heat) are so-called mean-field exponents which do not correspond to realistic systems (three or two dimensional), rather they describe the limit of high-dimensions.

In order to compare the mean-field results which we obtained so far with a better approximation let us turn to the classical limit of the Heisenberg model. In the classical limit, $S \rightarrow \infty$, the Brillouin function goes over to the Langevin function

$$L(x) = \coth(x) - \frac{1}{x}, \quad (9)$$

leading ones again to a self-consistency equation which can be solved numerically.

3 Classical limit and Monte Carlo simulation

In the classical limit the spins are simply three dimensional classical vectors of constant length and a good numerical approach to calculate thermal equilibrium properties is the Monte Carlo method [13]. Within a Monte Carlo approach trajectories in phase space are calculated following a master equation [14] for the time development of the probability distribution $P_s(t)$ in phase space,

$$\frac{dP_s}{dt} = \sum_{s'} (P_{s'} w_{s' \rightarrow s} - P_s w_{s \rightarrow s'}). \quad (10)$$

Here, S and S' denote different states of the system and the w are the transition rates from one state to another one which have to fulfill the detailed balance condition [14],

$$\frac{w_{s \rightarrow s'}}{w_{s' \rightarrow s}} = \exp\left(\frac{E(S) - E(S')}{k_B T}\right). \quad (11)$$

The master equation describes the coupling of the system to the heat bath [14]. Within the Monte Carlo method trajectories in phase space following Eq. 10 are calculated usually using

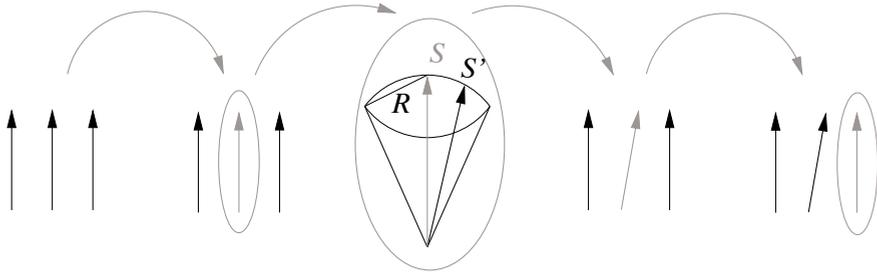


Fig. 2: Illustration of a Monte Carlo single spin flip algorithm in a three-spin system: 1) we start with some initial condition 2) one spin is selected 3) a trial step is made (here a small deviation from the initial state) 4) in this example the trial step is accepted 5) another spin is selected

single-spin-flip dynamics (illustrated in Fig. 2). A single-spin-flip algorithm is performed in the following way: at the beginning one single spin from the lattice is chosen either randomly or in some systematic order and a trial step of this selected spin is made (possible choices for trial steps will be described in detail below). Then the change of the energy of the system is computed according to the Hamiltonian of the system (in our case Eq. 1). Finally the trial step is accepted, for instance with the heat-bath probability,

$$w_{s \rightarrow s'} = \frac{w_0}{1 + \exp\left(\frac{E(S') - E(S)}{k_B T}\right)}, \quad (12)$$

which is one possible choice among others satisfying the condition Eq. 11 for any arbitrary constant w_0 . Scanning the lattice and performing the procedure explained above once per spin (on average) is called one Monte Carlo step (MCS). It defines a quasi-time scale of the simulation. The connection to real time — if there is one at all — is in general an open problem which is settled up to now only in certain cases [15]. The way the trial step is chosen is of importance for the efficiency of the algorithm as well as for the physical interpretation of the dynamic behavior of the algorithm [16]. One possible trial step among others which is often used in models with continuous degrees of freedom is a small deviation from the initial state (see Fig. 2). For a classical spin this could be a movement of the spin with uniform probability distribution within a given opening angle around the initial spin direction.

Trial steps for Monte Carlo algorithms have to fulfill two necessary conditions: they have to be ergodic and symmetric. Ergodicity demands that time averages yield identical results as ensemble averages. Thus it must be guaranteed that the whole phase space can be sampled by an algorithm. An example for a non-ergodic algorithm in a Heisenberg model is $S_z \rightarrow -S_z$. Here, starting from some initial condition the spin can only reach two positions out of the whole phase space which is a unit sphere for a classical Heisenberg spin. Nevertheless, one is allowed to perform such reflection steps as long as one uses *also* other trial steps that guarantee ergodicity. These ideas lead to combinational algorithms which — depending on the problem — can be very efficient [17]. The second condition which has to be fulfilled by any algorithm is a symmetry condition: for the probability to do a certain trial step it must be $p_t(s \rightarrow s') = p_t(s' \rightarrow s)$. Otherwise Eq. 11 is not fulfilled since the probabilities to perform certain trial steps contribute to the transition rates. The symmetry condition would for instance be violated in a

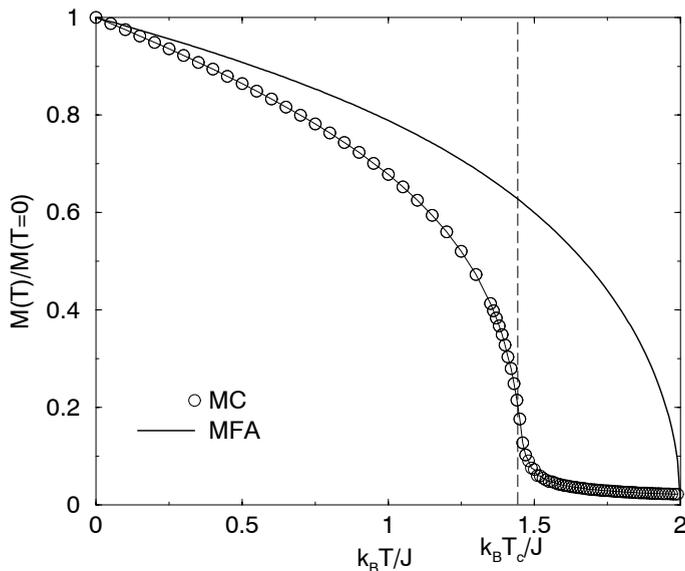


Fig. 3: Temperature dependence of the magnetization in the classical limit [10]. Shown is a comparison of the mean-field solution with the more accurate results from Monte Carlo simulations.

Heisenberg system if one chooses new trial spin directions by simply generating three random numbers as S_x , S_y , and S_z coordinates within a cube and normalizing the resultant vector to unit length. Before normalization the random vectors are homogeneously distributed within the cube but after the normalization they have some non-uniform probability distribution on the unit sphere which is higher along the diagonal directions of the cube. Hence, trial steps from any other direction into the diagonal direction are more probable than the other way round and the algorithm yields wrong results.

In Fig. 3 mean-field results (as in Fig. 1) for the classical limit are compared with results from Monte Carlo simulations. The Monte Carlo results are from a simulations of a simple cubic $32 \times 32 \times 32$ lattice with periodical boundary conditions where 100000 MCS were made for each data point. A single-spin flip algorithm was used with the trial step as explained above. One can clearly see so-called finite size effects [13] coming from the fact that the simulated lattice is not infinite, leading to the rounding of the magnetization close to T_c . The real T_c of an infinite system is close to the inflection point of the magnetization curve. Apart from these finite-size effects close to T_c the Monte Carlo results are practically exact. As one can see the mean-field approximation overestimates T_c strongly. The best known estimate of T_c (from Monte Carlo simulations using a cluster algorithm and a finite-size scaling analysis) is $T_c = 1.4427 \pm 0.0002$ and that of the critical exponent β is $\beta = 0.328 \pm 0.001$ [18].

4 Three dimensional magnets: RPA

In this chapter we will go beyond mean-field theory and calculate the temperature dependent magnetization of a three dimensional quantum Heisenberg model using the theory of Tjablykov [19]. In order to give just a brief overview we start with a Hamiltonian neglecting the Zeeman energy

$$\mathcal{H} = -\frac{1}{2\hbar^2 S^2} \sum_{i,j} J_{ij} \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j \quad (13)$$

but without the restriction to nearest neighbors so that J_{ij} stands for the exchange interaction between any sites i and j . For simplicity we will do the calculation for a $S = 1/2$ system since then it is

$$\tilde{S}_i^+ \tilde{S}_i^- = \hbar \left(\frac{\hbar}{2} + \tilde{S}_i^z \right) \quad (14)$$

so that in order to calculate the magnetization it is sufficient to calculate the thermal expectation value of the left term (for a more general treatment see [6]). For that we use the retarded Green's function (for an introduction to the Green's functions method see the appendix in [6]),

$$G_{ij}^{\text{ret}} = \langle \langle \tilde{S}_i^-(t); \tilde{S}_i^+(t') \rangle \rangle^{\text{ret}} = -i\theta(t-t') \langle [\tilde{S}_i^-(t), \tilde{S}_i^+(t')] \rangle. \quad (15)$$

Here, the operators are in the Heisenberg representation,

$$S_i^\pm(t) = e^{\frac{i}{\hbar}\mathcal{H}t} S_i^\pm e^{-\frac{i}{\hbar}\mathcal{H}t}.$$

For the energy representation (Fourier transform) of this Green's function,

$$G_{ij}^{\text{ret}}(E) = \int_{-\infty}^{\infty} d(t-t') e^{\frac{i}{\hbar}E(t-t')} G_{ij}^{\text{ret}}, \quad (16)$$

the following equation of motion can be derived,

$$EG_{ij}^{\text{ret}}(E) = -2\hbar^2 \delta_{ij} \langle \tilde{S}_i^z \rangle + \sum_m \frac{4J_{im}}{\hbar} \left(\langle \langle \tilde{S}_m^- \tilde{S}_i^z; \tilde{S}_j^+ \rangle \rangle^{\text{ret}} - \langle \langle \tilde{S}_i^- \tilde{S}_m^z; \tilde{S}_j^+ \rangle \rangle^{\text{ret}} \right). \quad (17)$$

This equation is still exact but it can hardly be solved because it combines a Green's function on the left hand side with higher order Green's functions on the right hand side. One could now derive an equation of motion for the Green's functions on the right hand side but this would lead to even higher order Green's functions, and so on.

One famous approximation to solve this problem is after Tjablykov [19] (also called RPA, random phase approximation) where we set

$$\langle \langle \tilde{S}_m^- \tilde{S}_i^z; \tilde{S}_j^+ \rangle \rangle^{\text{ret}} \rightarrow \langle \tilde{S}_i^z \rangle \langle \langle \tilde{S}_m^-; \tilde{S}_j^+ \rangle \rangle^{\text{ret}} \quad \text{and} \quad \langle \langle \tilde{S}_i^- \tilde{S}_m^z; \tilde{S}_j^+ \rangle \rangle^{\text{ret}} \rightarrow \langle \tilde{S}_i^z \rangle \langle \langle \tilde{S}_i^-; \tilde{S}_j^+ \rangle \rangle^{\text{ret}}. \quad (18)$$

In some sense this is like a mean-field approximation where an operator \tilde{S}_i^z is replaced by its thermal average (compare e. g. Eqs. 1 and 4). However, here this is done in the equation of motion and not in the Hamiltonian. We will see that this leads indeed to better results.

With the approximation above and assuming once again translational invariance (that $\langle \tilde{\mathbf{S}}_i \rangle$ is identical everywhere in the lattice) the equation of motion simplifies to

$$\left(E + \frac{4\langle \tilde{S}_i^z \rangle}{\hbar} J(0) \right) G_{ij}^{\text{ret}}(E) = -2\hbar^2 \delta_{ij} \langle \tilde{S}_i^z \rangle + \frac{4\langle \tilde{S}_i^z \rangle}{\hbar} \sum_m J_{im} G_{mj}^{\text{ret}}(E). \quad (19)$$

The solution of this equation can be obtained by a Fourier transform leading to

$$G_{\mathbf{q}}^{\text{ret}}(E) = \frac{-2\hbar^2 \langle \tilde{S}_i^z \rangle}{E - E(\mathbf{q}) + i0^+} \quad (20)$$

with

$$E(\mathbf{q}) = \frac{4\langle \tilde{S}_i^z \rangle}{\hbar} (J(0) - J(\mathbf{q})). \quad (21)$$

The poles of the Green's function are the energy excitations of the system where $J(\mathbf{q})$ is the Fourier transform of the exchange coupling constants,

$$J(0) - J(\mathbf{q}) = \frac{1}{N} \sum_{ij} J_{ij} (1 - e^{i\mathbf{q}\cdot\mathbf{r}}) \sim q^2. \quad (22)$$

In the equation above the last term is an approximation for small q , i. e., low energy which later on will turn out to be important for the understanding of the low temperature behavior. A very similar result can be derived within the framework of spin wave theory where the energy excitations are called magnons [6, 20]. The only difference is that following spin wave theory simply the spin quantum number S is in the pre-factor of Eq. 21 instead of its thermal average $\langle \tilde{S}_i^z \rangle$.

Using the spectral theorem one obtains

$$\langle \tilde{S}_i^+ \tilde{S}_j^- \rangle = \frac{1}{N} \sum_{\mathbf{q}} e^{-i\mathbf{q}(\mathbf{R}_i - \mathbf{R}_j)} \frac{2\hbar \langle \tilde{S}_i^z \rangle}{\exp(E(\mathbf{q})/k_B T) - 1} \quad (23)$$

and using Eq. 14 for the case $i = j$ we can derive an equation for the magnetization,

$$\langle \tilde{S}_i^z \rangle = \frac{\hbar}{2} \left(1 + \frac{2}{N} \sum_{\mathbf{q}} \frac{1}{\exp(E(\mathbf{q})/k_B T) - 1} \right)^{-1}. \quad (24)$$

Note, that this is once again a self consistency equation as earlier in our mean-field calculations since $E(\mathbf{q})$ contains also $\langle \tilde{S}_i^z \rangle$ (see Eq. 21). For a numerical evaluation a continuum version can be derived [6], namely

$$\frac{\hbar}{2\langle \tilde{S}_i^z \rangle} = \frac{V}{N(2\pi)^3} \int d^3q \coth \left(\frac{2\langle \tilde{S}_i^z \rangle (J(0) - J(\mathbf{q}))}{\hbar k_B T} \right), \quad (25)$$

which can be solved as before by a root finding program where the integral and — depending on the assumptions about the J_{ij} also $J(\mathbf{q})$ — has to be calculated numerically.

A numerical solution of the equation above is shown in Fig. 4. These data were calculated for a simple cubic lattice with nearest neighbor interaction only. The magnetization behaves like an order parameter of a ferromagnetic transition with a T_c which is clearly smaller than that of a mean-field approximation. We argued already in connection with Fig. 3 that mean-field theory overestimates T_c and we will see later that the lower T_c from RPA is indeed more realistic.

For low temperatures Eq. 24 can be expanded, in the continuum version leading to

$$\begin{aligned} \Delta m = \frac{\hbar}{2} - \langle \tilde{S}_i^z \rangle &\sim \int d^3q \frac{1}{\exp(E(\mathbf{q})/k_B T) - 1} \\ &\sim \int dE \frac{D(E)}{\exp(E/k_B T) - 1}. \end{aligned} \quad (26)$$

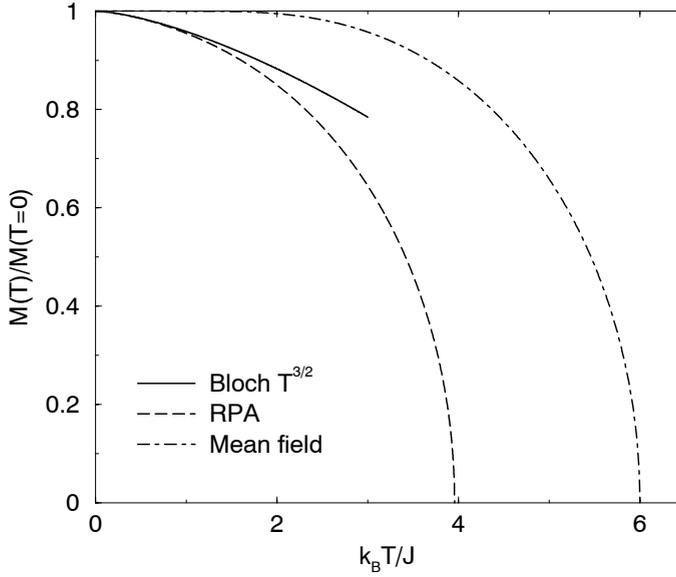


Fig. 4: Temperature dependence of the reduced magnetization in RPA approximation for a simple cubic lattice with $S = 1/2$ [10]. For comparison the corresponding mean-field solution is also shown. The solid line is Bloch's $T^{3/2}$ law.

Here, $D(E)$ is the density of states which depends on the dimension of the system and will be discussed in the next chapter. For three dimensions and low temperatures (small q) it is $E(q) \sim q^2$ (see Eq. 22) and $D(E) \sim \sqrt{E}$ so that we obtain

$$\Delta m \sim \int dE \frac{\sqrt{E}}{\exp(E/k_B T) - 1} \sim T^{3/2}. \quad (27)$$

This is Bloch's famous $T^{3/2}$ law [21] which means that with increasing temperature the magnetization decreases from its ground state value proportion to $T^{3/2}$. This is also true for other spin quantum numbers. The according curve is also shown in Fig. 4. Note, that the mean-field theory does not yield Bloch's $T^{3/2}$ law. A low temperature expansion of the mean-field self consistency equation (Eq. 5) shows that here the low temperature deviation of the magnetization grows exponentially.

Similar calculations can also be done for other spin quantum numbers. Numerical results are shown in the graph on the left hand side of Fig. 5. As in mean-field theory, the magnetization curves depend on the spin quantum number. Especially, from an expansion of Eq. 25 one can derive an analytical expression for the critical temperature. Close to T_c the magnetization is small so that the coth can be expanded leading to

$$k_B T_c = \frac{N(S+1)}{3S} \left(\sum_{\mathbf{q}} \frac{1}{(J(0) - J(\mathbf{q}))} \right)^{-1}. \quad (28)$$

If we restrict ourselves to nearest neighbor interaction and calculate the sum numerically for different lattice types we obtain [5]

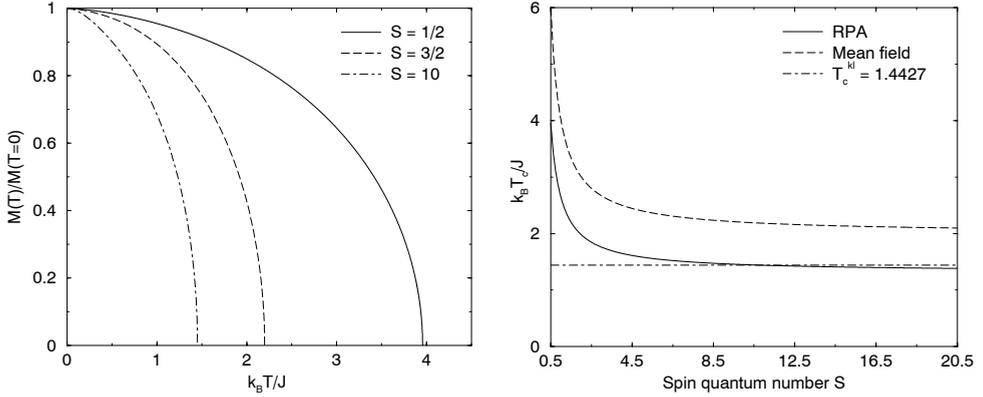


Fig. 5: left panel: Temperature dependence of the reduced magnetization in RPA approximation for a simple cubic lattice with different quantum numbers S [10]; right panel: comparison of critical temperature versus quantum number from mean-field theory, RPA and the best known value of the classical limit.

$$k_B T_c = \frac{zJ(S+1)}{3S} \cdot \begin{cases} 0.660 & \text{s.c.} \\ 0.718 & \text{b.c.c.} \\ 0.744 & \text{f.c.c.} \end{cases} \quad (29)$$

where z is once again the number of nearest neighbors in the respective lattice. Comparing this result once again with the mean-field result (Eq. 6) one can see that the structure of the equation is the same. However, the numerical factor of mean-field theory is equal to one and, furthermore, there is also a qualitative difference since in mean-field theory the lattice structure is not relevant while in RPA the lattice structure matters.

The graph on the right hand side of Fig. 5 compares mean-field and RPA results for the critical temperatures for a simple cubic lattice with nearest neighbor interaction. For large spin quantum number the RPA result is close to — but not identical with — the best known numerical value for a classical system which is also shown in the figure.

5 Magnetism in lower dimensions

Within mean-field approximation there is always a phase transition to ferromagnetic order in the Heisenberg model, no matter whether we have a one, two or three dimensional system. But is this really true? We will show now that this is not the case.

An influence of the dimension of the system within RPA can be seen in Eq. 26 which is a low temperature approximation for the influence of thermal excitations which lead to a deviation of the magnetization from its ground state. These are expressed as an integral which indeed depends on the dimension.

With the density of states

$$D(E)dE = \begin{cases} 2\pi q dq & \text{in two dimensions} \\ dq & \text{in one dimension} \end{cases} \quad (30)$$

and using once again the low temperature approximation $E \sim q^2$ (see Eq. 22) one obtains

$$D(E) \sim \begin{cases} \text{const} & \text{in two dimensions} \\ E^{-1/2} & \text{in one dimension} \end{cases} \quad (31)$$

so that the integral

$$\Delta m \sim \int_0^\infty dE \frac{D(E)}{\exp(E/k_B T) - 1} \rightarrow \infty \quad (32)$$

diverges in both, two and one dimensions. This means that low energy excitations which occur for low temperatures lead already to “infinite” deviations from the ground state which is a strong argument that no thermally stable magnetic order occurs on one and two dimensions. In other words, it is $T_c = 0$. This fact can also be proven rigorously and is more accurately formulated in the famous [22, 20]

Mermin-Wagner theorem:

There is no spontaneous long-range ferromagnetic order for isotropic Heisenberg models with short-range interaction ($\sum_j J_{ij} r_{ij}^2 < \infty$).

In this theorem there are two restrictions. One concerns the range of interactions and there is indeed one physically relevant magnetic interactions which decays slower and is long-range in that sense, namely the dipole - dipole interaction. Even though this interaction is usually much smaller than the exchange it can be relevant since it decays with the distance r like $J(r) \sim r^{-3}$ so that the sum over the interaction diverges,

$$\sum_j J_{ij} \sim \int_{\Delta r}^\infty r^2 dr \frac{1}{r^3} \rightarrow \infty.$$

The second restriction is isotropy and indeed, often magnetic systems are anisotropic, since even the lattice structure (via spin orbit coupling) can lead to the fact that certain crystallographic axes may be energetically favorable for the spin orientation. These anisotropies are often taken care of by including additional terms in the Hamiltonian, e. g. in form of a uniaxial anisotropy. The complete Hamiltonian then reads

$$\mathcal{H} = -\frac{1}{2\hbar^2 S^2} \left(\sum_{i,j} J_{ij} \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j + 2K \sum_i (\tilde{S}_i^z)^2 \right). \quad (33)$$

Here, spin directions along the z axis of the system are energetically favored by the second term and K is called anisotropy constant. Any anisotropy changes the critical behavior of a system drastically since it breaks a symmetry. For small anisotropies an estimate of the K dependence of the critical temperature $T_c(2D)$ of a two dimensional system was derived by Bander and Mills [23],

$$T_c(2D) = T_c(3D) / \ln \left(\frac{3\pi k_B T_c(3D)}{4K} \right) \quad (34)$$

using renormalization group theory. This result is shown in Fig. 6. T_c vanishes in the isotropic limit ($K \rightarrow 0$) in accordance with the Mermin-Wagner theorem. Interestingly, for finite K

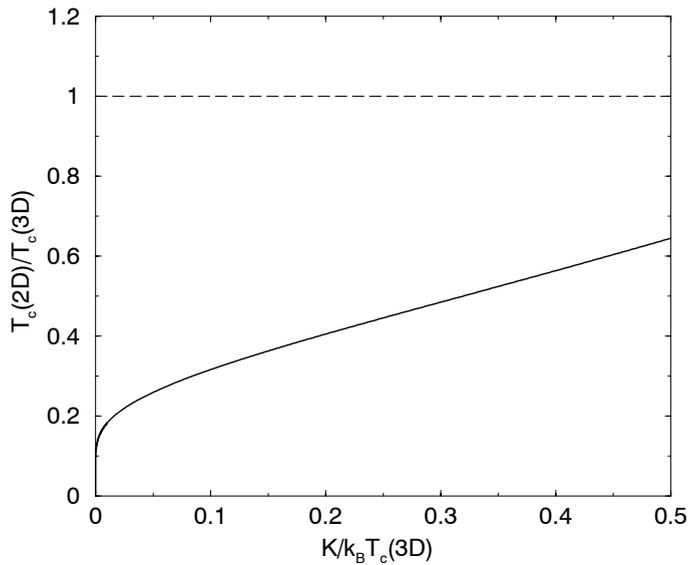


Fig. 6: Critical temperature of a two dimensional system versus anisotropy following Eq. 34.

there is a rapid increase of T_c reaching reasonable values (say 20% of the critical temperature in three dimensional systems) for anisotropy values of only a few % of the ferromagnetic coupling constant.

For any finite anisotropy value the two dimensional Heisenberg model shows a ferromagnetic phase transition with a finite T_c . In terms of universality the Heisenberg model with any finite anisotropy value is in the universality class of the Ising model. The Ising model is a classical Heisenberg model in the limit of infinite anisotropy so that only two possible states for each spin remain (say spin-up and spin-down) [7]. Hence, the dimension of the spin is reduced to one instead of three for the Heisenberg model. In fact, for the two dimensional Ising model there exists even an analytic solution and the Curie temperature ($k_B T_c = 2.269185J$ for a square lattice) as well as the critical exponents (e. g. $\beta = 1/8$, $\gamma = 7/4$) have been calculated exactly [24, 20]. In one dimension even the Ising model does not show long-range order at finite temperatures [7].

6 Summary

In this lecture we focused on the temperature dependence of ferromagnetic order. We did this within the framework of the Heisenberg model using different approximations.

The mean-field theory provides a first understanding of the ferromagnetic phase transition and a first estimate of the Curie temperature. However, mean-field theory overestimates the tendency for long-range order. The estimate of the Curie temperature is too high and, furthermore, a phase transition is also suggested in less than three dimensions where the Heisenberg model in fact shows no thermally stable long-range order.

In the classical limit Monte Carlo methods can be used to calculate thermal equilibrium prop-

erties. Apart from finite-size effects and — depending on the model — possible problems with the equilibration time (\rightarrow computation time), the results from a Monte Carlo simulation are practically exact so that one can also calculate critical exponents. Since the latter are universal these critical exponents are also relevant for quantum spin systems.

The theory of Tjablykov (RPA) provides a better estimate of the critical temperature as compared to mean-field theory. Furthermore Bloch's $T^{3/2}$ law (which is a purely quantum mechanical low-temperature result) can be derived within this context. Also the results suggest that no magnetic long-range order can occur in a one or two dimensional isotropic Heisenberg model. This was also proven rigorously by Mermin and Wagner.

However, in a two dimensional Heisenberg model with an additional anisotropy magnetic order can occur. For any finite value of the anisotropy constant the Heisenberg model falls into the Universality class of the Ising model where a phase transition occurs at finite temperatures in two dimensions but not in one dimension.

The understanding of thermal effects in low dimensional systems is an ongoing area of research. It is still an open question in how far an experimental system can be low dimensional. How small does it have to be, what does the crossover from bulk to lower dimensional behavior look like, and what other related effects can occur? Is a film with a thickness of a few atomic layers two dimensional? And what would we expect then, no magnetic long-range order at finite temperatures due to the Mermin-Wagner theorem or is there always "some" anisotropy so that magnetic order is stabilized. What critical exponents will we see, really those of the Ising model? Can we calculate T_c theoretically for a given material and film thickness? Scientists have worked on many of these problems but there are still lots of open questions and there is much more work to be done along these lines.

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