1 The Heisenberg model

1.1 Definition of the model

The model we will focus on is called the Heisenberg model. It has the following Hamiltonian:

$$\mathcal{H} = \frac{1}{2} \sum_{\substack{i,j\\i \neq j}} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{1}$$

Here i and j refer to sites on a lattice. The model can be defined on any lattice, but for concreteness (and to keep things simple) we will here limit ourselves to a hypercubic lattice in d dimensions (d = 1, 2, 3).^{1,2} The S_i are spin operators which live on the lattice sites. Spin components on the same lattice site obey the standard angular momentum commutation relations

$$[S_j^{\alpha}, S_j^{\beta}] = i \sum_{\gamma} \epsilon_{\alpha\beta\gamma} S_j^{\gamma} \quad (\alpha, \beta, \gamma = x, y, z)$$
 (2)

and spins on different sites commute with each other. The spin operators all have spin S, i.e. the operators S_i^2 have eigenvalue S(S+1) where S is an integer or half-integer. The spin interaction in (1), which is of the form $S_i \cdot S_j$, is called an **exchange interaction**, and the coefficients J_{ij} are called **exchange constants**. We will make the simplifying assumption (which is often realistic) that the spin interactions are negligible between spins that are not nearest-neighbors, i.e. J_{ij} is nonzero only if i and j are nearest-neighbor lattice sites, in which case we further assume $J_{ij} = J$, where J is a constant. There are then two different cases to consider, J < 0 and J > 0. For J < 0 the interaction energy of two spins favors them to be parallel; this is the ferromagnetic case. For J > 0 antiparallel orientation is instead favored; this is the antiferromagnetic case.

1.2 The S=1/2 Heisenberg antiferromagnet as an effective low-energy description of the half-filled Hubbard model for $U\gg t$

It turns out that the magnetic properties of many insulating crystals can be quite well described by Heisenberg-type models of interacting spins. Let us consider an example based on assuming that the electrons can be described in terms of the so-called Hubbard model, with Hamiltonian

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}.$$
 (3)

This is probably the most important (and famous) lattice model of interacting electrons. $c_{i\sigma}^{\dagger}$ creates an electron on site i with spin σ , and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ counts the number of electrons with spin σ on site i. In this model there is therefore one electronic orbital per site. The first term in (3) is the kinetic energy describing electrons hopping between nearest-neighbor sites i and j, and the second term is the interaction energy describing the energy cost U > 0

¹In 2 dimensions a hypercubic lattice is a square lattice and in 3 dimensions it is a cubic lattice.

²Periodic boundary conditions will be used in all spatial directions, so that the Hamiltonian is fully translationally invariant.

associated with having two electrons on the same site (these electrons must have opposite spin, as having two electrons on the same site with the same spin would violate the Pauli principle). Note that the interaction energy between electrons which are not on the same site is completely neglected in this model. The Hubbard model is the simplest model describing the fundamental competition between the kinetic energy and the interaction energy of electrons on a lattice. Despite much research, there is still a great deal of controversy about many of its properties in two and three dimensions (the model has been solved exactly in one dimension, but even in that case the solution is extremely complicated).

1.2.1 Physical picture

Now consider the case when there is exactly N/2 spin-up electrons and N/2 spin-down electrons in the system, where N is the number of lattice sites. Hence the total number of electrons is N which equals the number of lattice sites. This is called the half-filled case because maximally the system could contain two electrons per site (one of each spin) and thus a total electron number of 2N. Assume further that $U \gg t$. This suggests that to find the low-energy states we should first minimize the interaction energy and then treat the kinetic energy as a perturbation. The interaction energy is minimized by putting exactly one electron on each site; then no site is doubly occupied so the total interaction energy is zero. Moving an electron creates a doubly occupied site which is penalized by a large energy cost U. Thus as long as we're only interested in understanding the physics of the system for energies (and/or temperatures) much less than U, we can neglect configurations with double occupancies. Thus the interaction energy completely determines the charge distribution of the electrons. What about the spin distribution, i.e. how to put up- and down-spin electrons relative to each other? As far as the interaction energy is concerned, any spin distribution gives the same energy. However, if we now consider the kinetic energy term $(\propto t)$ as a perturbation, it is clear that (see Fig. 1(a)) if neighboring electrons have opposite spins, an electron can hop (virtually, in the sense of 2nd order perturbation theory) to a neighboring site and back; this virtual delocalization reduces the kinetic energy. In contrast (see Fig. 1(b)), if neighboring spins are parallel such hopping is forbidden, as the intermediate state with two electrons on the same site with the same spin would violate the Pauli principle. Therefore in this situation an effective interaction is generated which favors neighboring electrons to have opposite spin, i.e. antiparallel orientation. It can be shown⁴ that the resulting effective model, valid at temperatures and energies $\ll U$, is the Heisenberg antiferromagnet for the S=1/2 electron spins, with $J = 4t^2/U$ (this expression for J can be understood from 2nd order perturbation theory: there is one factor of -t for each of the two hops (first to the neighboring site, then back) and a factor U coming from the energy denominator due to the larger energy of the intermediate state). Therefore, the antiferromagnetic exhange interaction J comes about due to an interplay between electron hopping, the electron-electron interactions, and the Pauli principle; the effect of the antiferromagnetic exchange is to reduce the kinetic energy of the electrons.

³That the kinetic energy is reduced by this process can be understood from the formula for the energy correction in 2nd order perturbation theory, which is always negative for the ground state.

⁴See e.g. Auerbach, "Interacting electrons and quantum magnetism," Secs. 2.3 and 3.2, or Nagaosa, "Quantum field theory in strongly correlated electronic systems," Sec. 3.1.

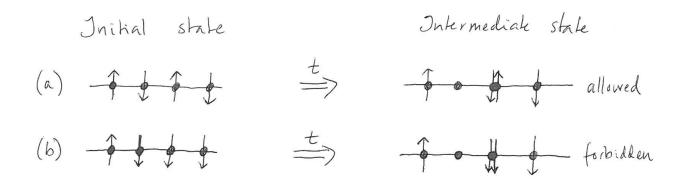
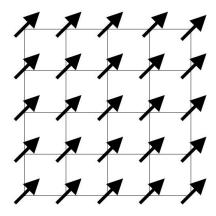


Figure 1: Illustration of why an effective antiferromagnetic interaction is generated in the half-filled Hubbard model with $U \gg t$. In both (a) and (b) the transition shown is between an initial state with an electron on each site and an intermediate state where the electron initially on site 2 has hopped to site 3. See text for further explanation.

We will not here go into how other examples of Heisenberg models (e.g. with spin S > 1/2 on each site and/or with ferromagnetic interactions) can arise as low-energy descriptions of different systems. Thus in the remainder of these notes we will simply consider the Heisenberg model as an interesting effective model of interacting spins and explore its properties (such as the nature of its ground state and excitations) without dwelling more on the origin of the model itself.

1.3 Ferro- and antiferromagnetic order

Let us discuss the behavior of the spins, as a function of temperature, in materials described by the Heisenberg model. At high temperatures there are strong thermal fluctuations so that the spins are disordered, meaning that the expectation value of each spin vanishes: $\langle S_i \rangle = 0$. (Here the brackets represent both a thermal and quantum-mechanical expectation value.) However, below some critical temperature T_c it may be that the spins order magnetically, meaning that the spins on average point in some definite direction in spin space, $\langle S_i \rangle \neq 0$. Whether or not such magnetic order occurs depends on the dimensionality and type of lattice, and the range of the interactions (we will limit ourselves to hypercubic lattices and nearestneighbor interactions in our explicit investigation of the Heisenberg model). If magnetic order occurs with $T_c > 0$, then, as the temperature is lowered from T_c down to zero, $\langle S_i \rangle$ will increase and reach some maximum value at zero temperature. The critical temperature T_c is called the Curie temperature (T_C) in ferromagnets and the Neel temperature (T_N) in antiferromagnets. The spin ordering pattern in two magnetically ordered phases are illustrated for a square lattice in Fig. 2: In the ferromagnetic case (J < 0) all spins point in the same direction (Fig. 2(a)) while in the antiferromagnetic case (J>0) neighboring spins point in opposite directions (Fig. 2(b)).



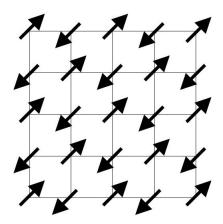


Figure 2: Average spin directions in phases with (a) ferromagnetic and (b) antiferromagnetic order on the square lattice. (The ordering direction is arbitrary.)

2 The Holstein-Primakoff representation

Note that the commutator of two spin operators is itself an operator (see (2)), rather than just a complex number (c-number). This makes it much more complicated⁵ to work directly with spin operators than with canonical bosonic (fermionic) creation and annihilation operators whose commutators (anticommutators) are just c-numbers. It would therefore be advantageous if one could represent the spin operators in terms of such canonical bosonic or fermionic operators and work with these instead. Fortunately quite a few such representations are known. In these lectures we will make use of the so-called Holstein-Primakoff (HP) representation which expresses the spin operators on a site j in terms of canonical boson creation and annihilation operators a_i^{\dagger} and a_j as follows:

$$S_{j}^{+} = \sqrt{2S - \hat{n}_{j}} a_{j},$$
 (4)
 $S_{j}^{-} = a_{j}^{\dagger} \sqrt{2S - \hat{n}_{j}},$ (5)
 $S_{j}^{z} = S - \hat{n}_{j}.$ (6)

$$S_i^- = a_i^\dagger \sqrt{2S - \hat{n}_i}, \tag{5}$$

$$S_i^z = S - \hat{n}_i. ag{6}$$

Here we have introduced the raising and lowering operators $S_j^{\pm} = S_j^x \pm i S_j^y$. The operator $\hat{n}_j \equiv a_j^{\dagger} a_j$ is the number operator for site j, i.e. it counts the number of bosons on this site. As the allowed eigenvalues of S_i^z are $-S, -S+1, \ldots, S$ you can see from the equation for S_i^z that this boson number must satisfy the constraint

$$\langle \hat{n}_j \rangle \le 2S.$$
 (7)

Also note that the expressions for S_j^+ and S_j^- are Hermitian conjugates of each other, as they should be. It can be shown that the spin commutation relations (2) and the relation

⁵At least as far as analytical (as opposed to numerical) approaches are concerned.

 $S^2 = S(S+1)$ follow from the HP representation and the bosonic commutation relations $[a_j, a_j^{\dagger}] = 1$ etc. (You will be asked to verify this in a tutorial). As will hopefully become clear in the next couple of sections, the HP representation is very useful for studying magnetically ordered states and their excitations. The reason for this is related to the fact that the vacuum of the a_j bosons (i.e. the state with no such bosons) is the state corresponding to the maximum eigenvalue S of S_j^z .

3 Spin-wave theory of ferromagnets

We will now begin our study of the Heisenberg model (1) using spin-wave theory. We will first consider the ferromagnetic case, with J < 0 (which can be written J = -|J|). It will be convenient to rewrite the Hamiltonian in terms of the raising and lowering operators $\hat{S}_j^{\pm} = \hat{S}_j^x \pm i \hat{S}_j^y$. Also since we're only considering nearest neighbor interactions we can write $j = i + \delta$ where δ is a vector connecting nearest-neighbor sites. Actually to avoid counting each interaction twice we will take δ to run over only half the nearest neighbor vectors. We will consider hypercubic lattices only. Thus in 1D, we take $\delta = +\hat{x}$, in 2D $\delta = +\hat{x}$, $+\hat{y}$ and in 3D $\delta = +\hat{x}$, $+\hat{y}$, $+\hat{z}$. This gives

$$\mathcal{H} = J \sum_{i,\delta} \left[\frac{1}{2} (S_i^+ S_{i+\delta}^- + S_i^- S_{i+\delta}^+) + S_i^z S_{i+\delta}^z \right]. \tag{8}$$

The state with all spins pointing along z, i.e. $S_j^z = S$ is a ground state of the Heisenberg ferromagnet. This should be intuitively quite reasonable, and it can be proven easily. First let us show that it is an eigenstate. When we apply (8) to this state, the part involving the ladder operators give exactly zero because the operators S_j^+ kill the ground state since it already has maximum S_j^z which therefore cannot be increased further. Acting with the $S_i^z S_j^z$ gives back an energy $-|J|S^2Nz/2$ times the same state, where z is the number of nearest neighbors. This shows that this state is an eigenstate. To show that it is also the ground state, we note that the minimal energy possible is given by

$$E_0 = -|J| \sum_{i,\delta} \max \langle \mathbf{S}_i \cdot \mathbf{S}_{i+\delta} \rangle. \tag{9}$$

It can be shown⁶ that $\max \langle \mathbf{S}_i \cdot \mathbf{S}_{i+\delta} \rangle = S^2$ which gives $E_0 = -|J|S^2Nz/2$, the same as above. Hence the state in question is indeed a ground state.

We will now use the HP representation to study the Heisenberg ferromagnet, especially its excitations. As noted earlier we will consider a hypercubic lattice in d spatial dimensions,

$$\langle O \rangle \equiv \langle \Psi | O | \Psi \rangle = \sum_{m,n} c_m^* c_n \underbrace{\langle \Phi_m | O | \Phi_n \rangle}_{O_n \delta_{mn}} = \sum_n |c_n|^2 O_n.$$

This shows that the largest value of $\langle O \rangle$ is given by the largest eigenvalue of O, obtained by taking $|\Psi\rangle$ to be the eigenstate of O with the largest eigenvalue.

⁶ The material in this footnote was not discussed in the lectures. Let O be a Hermitian operator and let $\{|\Phi_n\rangle\}$ be its complete set of orthonormal eigenstates, with eigenvalues O_n . We will consider the expectation value of O in an arbitrary state $|\Psi\rangle$. We can expand $|\Psi\rangle$ in the set $\{|\Phi_n\rangle\}$: $|\Psi\rangle = \sum_n c_n |\Phi_n\rangle$. Normalization of $|\Psi\rangle$ gives that $\sum_n |c_n|^2 = 1$. The expectation value of O can then be written

i.e. a standard lattice in one dimension, a square lattice in 2 dimensions, and a cubic lattice in 3 dimensions. The theory that will be developed is known as **spin-wave theory**.

A natural guess for the low-energy excitations would be that they just correspond to small collective oscillations of the spins around the ordering direction (which we choose to be the z direction). Thus these oscillations, which are called **spin waves**, make $\langle S_j^z \rangle$ less than the maximum value S. In terms of the HP representation this means that the boson number $\langle \hat{n}_j \rangle$ is nonzero, see (6). If this boson number $\langle \hat{n}_j \rangle$ is much smaller than S the reduction in S_j^z is small (i.e. very weak oscillations) and one might expect that an expansion in a small parameter proportional to $\langle \hat{n}_j \rangle / S$ would make sense. One might expect this to work better the larger S is, since one might guess that increasing S would make this parameter smaller (we'll verify this explicitly later). On the other hand, if it should turn out that $\langle \hat{n}_j \rangle / S$ is not small (this is something we'll have to check at the end of our calculation), then our basic assumption, that spin-waves are just weak oscillations around an ordered state, is wrong or at least questionable, and we may have to conclude that the system is not magnetically ordered after all. For example, this will be the conclusion if $\langle \hat{n}_j \rangle / S$ turns out to be divergent, which we'll see some examples of later.

The above indicates that spin-wave theory is essentially a 1/S expansion. It is semiclassical in nature, which follows since the limit $S \to \infty$ corresponds to classical spins, which can be seen e.g. from the fact that the eigenvalues of \hat{S}_i^2 are $S(S+1) = S^2(1+1/S)$. If the spins were just classical vectors of length S, the square of their length should be just S^2 . Instead we see that there is a correction factor (1+1/S) due to the quantum nature of the spins. As the correction factor goes to 1 in the limit $S \to \infty$, this limit corresponds to classical spins.

Let us now discuss the spin-wave theory for the Heisenberg ferromagnet in detail. As noted earlier, in both the quantum and classical ground state all the spins point along the same direction, which we will take to be the z direction. We then rewrite the spin operators in the Heisenberg Hamiltonian in terms of boson operators using the HP representation. We write $\sqrt{2S - \hat{n}_j} = \sqrt{2S}\sqrt{1 - \hat{n}_j/(2S)}$ and expand the last square root here in a series in the operator $\hat{n}_j/(2S)$. This gives

$$\mathcal{H} = -|J|NS^2z/2 - |J|S\sum_{i\,\boldsymbol{\delta}}[a_{i+\boldsymbol{\delta}}^{\dagger}a_i + a_i^{\dagger}a_{i+\boldsymbol{\delta}} - a_i^{\dagger}a_i - a_{i+\boldsymbol{\delta}}^{\dagger}a_{i+\boldsymbol{\delta}}] + O(S^0). \tag{10}$$

Here N is the total number of lattice sites and z is the number of nearest neighbors and

Now we consider spins on two different sites $i \neq j$. Since $(S_i + S_j)^2 = S_i^2 + S_j^2 + 2S_i \cdot S_j$, we can write

$$oldsymbol{S}_i \cdot oldsymbol{S}_j = rac{1}{2} \Big[(oldsymbol{S}_i + oldsymbol{S}_j)^2 - oldsymbol{S}_i^2 - oldsymbol{S}_j^2 \Big].$$

The largest expectation value of $S_i \cdot S_j$ is, from (6), given by the largest eigenvalue of the operator on the rhs of this equation. The three terms on the rhs commute with each other, so we can find simultaneous eigenstates for them. The eigenvalue of S_i^2 and S_j^2 is S(S+1). The eigenvalues of $S_i^2 + S_j^2 +$

$$\max \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \frac{1}{2} [2S(2S+1) - S(S+1) - S(S+1)] = S^2.$$

given by z=2d for a hypercubic lattice in d spatial dimensions. (Note that after doing the summations the two last terms inside the square brackets are in fact identical). We have only included terms of $O(S^2)$ and O(S) in (10). To this order, the HP representation reduces to $S_j^+ \approx \sqrt{2S}a_j$, $S_j^- \approx \sqrt{2S}a_j^\dagger$ (and $S_j^z = S - a_j^\dagger a_j$). The term of O(S) is quadratic in the boson operators and can be straightforwardly diagonalized. As it is quadratic it is equivalent to noninteracting bosons. Terms in the Hamiltonian which are higher order in the 1/S expansion (not shown) contain four or more boson operators and thus represent interactions between bosons. However, these are suppressed at least by a factor 1/S compared to the O(S) noninteracting term and one can thus hope that their effects are small (at least at large S and when the boson number is small) so that they can either be neglected to a first approximation or be treated as weak perturbations on the noninteracting theory.

Let us next diagonalize the quadratic, O(S) term. In this ferromagnetic case, this can be accomplished simply by introducing Fourier-transformed boson operators as follows:

$$a_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{i} e^{-i\mathbf{k} \cdot \mathbf{r}_{i}} a_{i}. \tag{11}$$

This is just a variable transformation, so there are as many operators a_k as there are operators a_i . The inverse transformation is

$$a_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i} a_{\mathbf{k}}.$$
 (12)

Periodic boundary conditions imply that e.g. $a_i = a_{i+N_x\hat{x}}$ where N_x is the number of sites in the x direction. This is satisfied if $e^{ik_xN_x} = 1$, i.e. k_x takes the form $k_x = 2\pi n_x/N_x$ where n_x is an integer. It is customary to choose n_x to take the N_x successive values $-N_x/2, -N_x/2+1, \ldots, N_x/2-1$ (here we have assumed for simplicity that N_x is even so that $N_x/2$ is in fact an integer). Then k_x takes values in the interval $[-\pi, \pi)$. Doing the same for all directions, the resulting values of k lie within what is called **the first Brillouin zone**. An important aspect of the transformation (11) is that it is canonical, i.e. it preserves the commutation relations in the sense that the operators a_k obey the same kind of commutation relations as the original boson operators: $[a_k, a_{k'}^{\dagger}] = \delta_{k,k'}$ etc. Inserting (12) in (10) and using that $\sum_i e^{i(k-k')\cdot r_i} = N\delta_{k,k'}$ one gets

$$\mathcal{H} = E_0 + \sum_{\mathbf{k}} \omega_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}, \tag{13}$$

where

$$E_0 = -|J|NS^2z/2 (14)$$

and

$$\omega_{\mathbf{k}} = 2|J|S\sum_{\delta} (1 - \cos \mathbf{k} \cdot \boldsymbol{\delta}) \equiv S|J|z(1 - \gamma_{\mathbf{k}}), \tag{15}$$

⁷Note that when the HP expressions for S_j^{\pm} are expanded in a series in $\hat{n}_j/(2S)$, and this series is truncated, the result is just approximate expressions for S_j^{\pm} . In particular they do not exactly obey the spin commutation relations.

where we have defined

$$\gamma_{\mathbf{k}} = \frac{2}{z} \sum_{\delta} \cos \mathbf{k} \cdot \delta. \tag{16}$$

Eq. (13) describes a Hamiltonian which is just a bunch of independent harmonic oscillators, each labeled by a wavevector \mathbf{k} . The quanta of the harmonic oscillators are called **magnons**; they are the quantized spin wave excitations (just like phonons are the quantized lattice vibrations in a crystal) with energy $\omega_{\mathbf{k}}$. In the limit $\mathbf{k} \to 0$, we have

$$\omega_{\mathbf{k}} \approx |J|S|\mathbf{k}|^2. \tag{17}$$

As a magnon with wavevector \mathbf{k} costs an energy $\omega_{\mathbf{k}} > 0$, the ground state has no magnons, i.e. $\langle \hat{n}_{\mathbf{k}} \rangle = 0$ at zero temperature (here $\hat{n}_k = a_k^{\dagger} a_k$). The ground state energy is therefore simply E_0 which is the interaction energy of all spins pointing in the same direction with maximal projection S along the z axis. As the temperature is increased, magnons will be thermally excited. Since they are just noninteracting bosons (when $O(S^0)$ terms and higher are neglected in the Hamiltonian, as done so far), the mean number of magnons with momentum \mathbf{k} is given by the Bose-Einstein distribution function,

$$\langle \hat{n}_{\mathbf{k}} \rangle = \frac{1}{e^{\beta \omega_{\mathbf{k}}} - 1}.\tag{18}$$

The magnetization $\mathbf{M} \equiv (1/N) \sum_i \langle \mathbf{S}_i \rangle$ is a natural measure of the strength of the putative magnetic order in the system (cf. the discussion in Sec. 1.3). If $M \equiv |\mathbf{M}|$ is positive (zero) we say that the system is (is not) ferromagnetically ordered. The larger M is, the stronger is the ferromagnetic order. We say that the magnetization is an **order parameter** for the ferromagnetic phase. By definition, an order parameter for a given type of order is a quantity that is nonzero in the phase(s) where that order is present and is zero in other phases. With the ordering direction being the z direction, we get

$$M = \frac{1}{N} \sum_{i} \langle S_{i}^{z} \rangle = S - \frac{1}{N} \sum_{i} \langle \hat{n}_{i} \rangle = S - \frac{1}{N} \sum_{k} \langle \hat{n}_{k} \rangle \equiv S - \Delta M.$$
 (19)

We'd like to look at how ΔM depends on temperature for low temperatures. We first introduce an artificial wavevector cutoff k_0 which is the smallest wavevector in the \mathbf{k} sum; the real system is described by the limit $k_0 \to 0$. We also introduce another wavevector $\bar{k} > k_0$ which is chosen such that $\omega_{\bar{k}} \ll k_B T \ll |J|S$; this means in particular that for $|k| < \bar{k}$ the quadratic form (17) is valid. This gives

$$\Delta M = \frac{1}{N} \left(\sum_{k_0 < |\mathbf{k}| < \bar{k}} \frac{1}{e^{|J|Sk^2/k_B T} - 1} + \sum_{|\mathbf{k}| > \bar{k}} \frac{1}{e^{\omega_{\mathbf{k}}/k_B T} - 1} \right).$$
 (20)

The second term is independent of k_0 and finite. For reasons that soon will become clear, we will therefore neglect it and focus on the first term. Converting the sum to an integral and expanding the exponential (using $|J|S^2k^2 \ll k_BT$) we get

$$\Delta M \propto \int_{k_0}^{\bar{k}} dk \ k^{d-1} \frac{k_B T}{|J| S k^2} \propto \frac{k_B T}{|J| S} \cdot \begin{cases} 1/k_0 + \dots, & d = 1 \\ -\log k_0 + \dots, & d = 2 \end{cases}$$
 (21)

⁸Here (and also in the antiferromagnetic case to be considered later) we gloss over a minor subtlety associated with the $\mathbf{k} = 0$ wavevector which comes with an energy $\omega_{\mathbf{k}} = 0$.

Therefore we see that, at nonzero temperatures in one and two dimensions, ΔM diverges as the cutoff k_0 is sent to zero. Therefore our initial assumption that this correction is small, is found to be wrong for these cases (note that the quantity $\Delta M/(2S)$ is the expectation value of the average over all sites of our original expansion parameter $\hat{n}_j/(2S)$, which we assumed to be small when we expanded the square roots in the HP expression). Thus we conclude that M=0 (i.e. there is no ferromagnetic order) at finite (i.e. nonzero) temperatures for the Heisenberg model in one and two dimensions.

For the case of three dimensions, it can be shown⁹ that $\Delta M \propto T^{3/2}$ as $T \to 0$. Thus spin-wave theory predicts that ferromagnetic order is stable (i.e. M > 0) at sufficiently low temperatures in three dimensions.

4 Spin-wave theory of antiferromagnets

We next turn to the antiferromagnetic case (J > 0 in (1)). As the ground state for classical spins has the spins on neighbouring sites pointing in opposite directions, one might naively guess that the ground state in the quantum case is analogous, thus having maximal and opposite spin projections $\pm S$ on neighboring sites. Such a state can be written

$$\prod_{j \in A} |S\rangle_j \prod_{l \in B} |-S\rangle_l \equiv |N\rangle. \tag{22}$$

Here A and B denote the two sublattices such that the spins on A (B) sites have spin projection S (-S), i.e. the states $|\pm S\rangle$ are eigenstates of S_z for the given lattice site with eigenvalue $\pm S$. It is however easy to see that $|N\rangle$ can not be the ground state, and is in fact not even an eigenstate, for the Heisenberg model for finite values of S: Acting with H in (1) on this state, the quantum fluctuation terms involving the spin raising and lowering operators change the state so that $H|N\rangle$ is not proportional to $|N\rangle$. Note that this did not happen in the ferromagnetic case because then the S^+ operators always killed the ferromagnetic ground

$$\frac{1}{e^x - 1} = e^{-x} \frac{1}{1 - e^{-x}} = e^{-x} \sum_{n=0}^{\infty} (e^{-x})^n = \sum_{n=1}^{\infty} e^{-nx},$$

and integrating over wavevectors up to infinity (i.e. $k_0 \to 0$ and $\bar{k} \to \infty$). This gives

$$\Delta M \approx \frac{1}{(2\pi)^3} \cdot 2 \cdot 2\pi \int_0^\infty dk \ k^2 \sum_{r=1}^\infty e^{-n|J|Sk^2/k_BT}.$$

Changing integration variable to $u = n|J|Sk^2/(k_BT)$ the integral to solve is $\int du \sqrt{u}e^{-u} = (1/2)\sqrt{\pi} \text{erf}(\sqrt{u}) - e^{-u}\sqrt{u}$ where erf is the so-called error function which satisfies erf(0) = 0 and $\text{erf}(\infty) = 1$. This gives finally

$$\Delta M \approx \frac{1}{8} \left(\frac{k_B T}{\pi |J| S} \right)^{3/2} \zeta(3/2),$$

where $\zeta(s) = \sum_{n} n^{-s}$ is the Riemann zeta function.

⁹ The material in this footnote was not covered in the lectures. In this case one can find the leading temperature dependence at low temperatures by writing the Bose-Einstein function in terms of a geometric sum as follows ($x \equiv |J|Sk^2/k_BT$):

state, leaving only the contribution from the S^zS^z part of the Hamiltonian. Consequently, quantum fluctuations play a much more important role in the antiferromagnetic case, as they change the ground state (and its energy) away from the "classical" result.

Although the ground state is not given by $|N\rangle$, it may still be that the ground state has antiferromagnetic order, i.e. that the spins on sublattice A point predominantly in one direction (taken to be the z direction here) and the spins on sublattice B point predominantly in the opposite direction. (If so the state $|N\rangle$ captures the structure of the true ground state at least in a qualitative sense.) To investigate this possibility we again develop a spin-wave theory based on expanding the square roots in the HP expansion. On the A sublattice where the spin projection in (22) is +S we use the standard expressions:

$$S_{Aj}^{+} = \sqrt{2S - a_j^{\dagger} a_j} a_j, \qquad (23)$$

$$S_{Aj}^{-} = a_j^{\dagger} \sqrt{2S - a_j^{\dagger} a_j}, \qquad (24)$$

$$S_{Aj}^z = S - a_j^{\dagger} a_j. \tag{25}$$

However, on the B sublattice where the spin projection in (22) is -S we must modify the HP expressions accordingly to reflect this:

$$S_{Bl}^{+} = b_l^{\dagger} \sqrt{2S - b_l^{\dagger} b_l}, \tag{26}$$

$$S_{Bl}^{-} = \sqrt{2S - b_l^{\dagger} b_l} b_l, \qquad (27)$$

$$S_{Bl}^z = -S + b_l^{\dagger} b_l. \tag{28}$$

Compared to the expressions on the A sublattice, these modified expressions correspond to the changes $S^+ \leftrightarrow S^-$, $S^z \to -S^z$, which preserve the commutation relations, which shows that the HP expressions for sublattice B are indeed correct. Note that different boson operators a_j and b_l have been introduced for sublattices A and B respectively. The indices j and l run over the sites in A and B respectively. Inserting the HP expressions in the Hamiltonian, expanding the square roots and keeping terms to order S in the Hamiltonian, we get

$$\mathcal{H} = J \sum_{j \in A} \sum_{\delta} \left[\frac{2S}{2} (a_j b_{j+\delta} + \text{h.c.}) + S(a_j^{\dagger} a_j + b_{j+\delta}^{\dagger} b_{j+\delta}) - S^2 \right]$$

$$+ J \sum_{l \in B} \sum_{\delta} \left[\frac{2S}{2} (b_l a_{l+\delta} + \text{h.c.}) + S(b_l^{\dagger} b_l + a_{l+\delta}^{\dagger} a_{l+\delta}) - S^2 \right].$$
(29)

Next we introduce Fourier-transformed operators

$$a_{\mathbf{k}} = \frac{1}{\sqrt{N_A}} \sum_{j \in A} e^{-i\mathbf{k} \cdot \mathbf{r}_j} a_j, \tag{30}$$

$$b_{\mathbf{k}} = \frac{1}{\sqrt{N_B}} \sum_{l \in B} e^{-i\mathbf{k} \cdot \mathbf{r}_l} b_l. \tag{31}$$

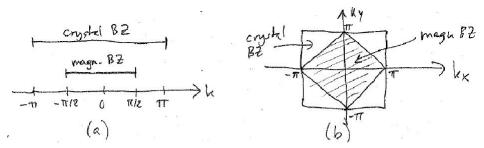


Figure 3: Crystal Brillouin zone and magnetic Brillouin zone in one dimension (a) and two dimensions (b).

where $N_A = N_B = N/2$ is the number of lattice sites in each sublattice. The inverse transformation is

$$a_j = \frac{1}{\sqrt{N_A}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_j} a_{\mathbf{k}}, \tag{32}$$

$$b_l = \frac{1}{\sqrt{N_B}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_l} b_{\mathbf{k}}. \tag{33}$$

The commutation relations are standard bosonic, i.e. the only nonzero commutators are $[a_{\mathbf{k}}, a_{\mathbf{k'}}^{\dagger}] = [b_{\mathbf{k}}, b_{\mathbf{k'}}^{\dagger}] = \delta_{\mathbf{k}, \mathbf{k'}}$. We choose the **k**-vectors to lie in the Brillouin zone associated with each sublattice. (Since the two sublattices are identical, their Brillouin zone is also identical). This Brillouin zone is called the magnetic Brillouin zone to distinguish it from the Brillouin zone associated with the full lattice which is called the crystal Brillouin zone. In one dimension periodic boundary conditions gives $a_{j+N_A\cdot 2\hat{x}}=a_j$ (the factor of 2 comes from the fact that the spacing between neighboring sites in the sublattice is 2, not 1) which gives $k_x = 2\pi n_x/(2N_A)$. Choosing the N_A values of n_x which lie closest to 0 (i.e. $n_x =$ $-N_A/2,\ldots,N_A/2-1$) then gives $k_x\in[\pi/2,\pi/2]$. Thus the length of the magnetic Brillouin zone is half the length of the crystal Brillouin zone $[\pi, \pi]$. In two dimensions the two sublattices are oriented at a 45 degree angle with respect to the full lattice and have a lattice spacing which is $\sqrt{2}$ larger. It follows from this that the magnetic Brillouin zone is a square oriented at a 45 degree angle with respect to the crystal Brillouin zone and has half its area. These facts are illustrated in Fig. 3. In the following you should keep in mind that when we are discussing antiferromagnets, it is implicitly understood that all k-sums are over the magnetic Brillouin zone.

Inserting (32)-(33) in the Hamiltonian and using $\sum_{j} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_{j}} = N_{A}\delta_{\mathbf{k},\mathbf{k}'}$ etc., and also renaming the summation variable \mathbf{k} as $-\mathbf{k}$ where needed, we get

$$\mathcal{H} = -NJS^2 z/2 + JSz \sum_{\mathbf{k}} [\gamma_{\mathbf{k}} (a_{\mathbf{k}} b_{-\mathbf{k}} + a_{\mathbf{k}}^{\dagger} b_{-\mathbf{k}}^{\dagger}) + a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}], \tag{34}$$

where $\gamma_{\mathbf{k}}$ was defined earlier in (16). While the last two terms in the O(S) part are in diagonal form, the first two terms are not; thus in contrast to the ferromagnetic case, Fourier transformation alone does not diagonalize the Hamiltonian in the antiferromagnetic case. To bring the Hamiltonian into diagonal form, we will perform another canonical transformation,

known as a Bogoliubov transformation:

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} b_{-\mathbf{k}}^{\dagger}, \tag{35}$$

$$\beta_{\mathbf{k}} = u_{\mathbf{k}} b_{\mathbf{k}} - v_{\mathbf{k}} a_{-\mathbf{k}}^{\dagger}. \tag{36}$$

Here $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are two real functions of \mathbf{k} which are to be determined. From the requirement that $[\alpha_{\mathbf{k}}, \alpha^{\dagger}_{\mathbf{k}'}] = [\beta_{\mathbf{k}}, \beta^{\dagger}_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}$ we get the condition

$$u_k^2 - v_k^2 = 1. (37)$$

From the requirement $[\alpha_{\mathbf{k}}, \beta_{\mathbf{k'}}] = 0$ we get another condition, $u_{\mathbf{k}}v_{-\mathbf{k}} = u_{-\mathbf{k}}v_{\mathbf{k}}$. This is satisfied if $u_{-\mathbf{k}} = u_{\mathbf{k}}$ and $v_{-\mathbf{k}} = v_{\mathbf{k}}$, which will be assumed to hold in the following. The inverse transformation is given by

$$a_{\mathbf{k}} = u_{\mathbf{k}} \alpha_{\mathbf{k}} + v_{\mathbf{k}} \beta_{-\mathbf{k}}^{\dagger}, \tag{38}$$

$$b_{\mathbf{k}} = u_{\mathbf{k}} \beta_{\mathbf{k}} + v_{\mathbf{k}} \alpha_{-\mathbf{k}}^{\dagger}. \tag{39}$$

By expressing the Hamiltonian in terms of the α and β bosons it can be rewritten as

$$\mathcal{H} = -NJS^2z/2 + JSz \sum_{\mathbf{k}} \{ (2\gamma_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}} + u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2)(\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^{\dagger}\beta_{\mathbf{k}}) + 2(\gamma_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}} + v_{\mathbf{k}}^2) + [\gamma_{\mathbf{k}}(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) + 2u_{\mathbf{k}}v_{\mathbf{k}}](\alpha_{\mathbf{k}}\beta_{-\mathbf{k}} + \alpha_{\mathbf{k}}^{\dagger}\beta_{-\mathbf{k}}^{\dagger}) \}.$$

$$(40)$$

Now we will choose $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ such that the term which is not on diagonal form, i.e. the term proportional to $\alpha_{\mathbf{k}}\beta_{-\mathbf{k}} + \alpha_{\mathbf{k}}^{\dagger}\beta_{-\mathbf{k}}^{\dagger}$, vanishes. Thus we require that

$$\gamma_{\mathbf{k}}(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) + 2u_{\mathbf{k}}v_{\mathbf{k}} = 0. \tag{41}$$

Furthermore we note that the condition (37) is automatically satisfied if we set

$$u_{\mathbf{k}} = \cosh \theta_{\mathbf{k}}, \quad v_{\mathbf{k}} = \sinh \theta_{\mathbf{k}}.$$
 (42)

Inserting this into (41) gives¹⁰ an equation which determines θ_k :

$$tanh 2\theta_k = -\gamma_k.$$
(43)

Since $\gamma_{-\mathbf{k}} = \gamma_{\mathbf{k}}$ it follows that $\theta_{-\mathbf{k}} = \theta_{\mathbf{k}}$ which is consistent with our earlier assumption that $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ were even functions of \mathbf{k} . Using (42) and (43), after some manipulations we get

$$\mathcal{H} = -NJS^{2}z/2 - NJSz/2 + \sum_{\mathbf{k}} \omega_{\mathbf{k}} (\alpha_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \beta_{\mathbf{k}}^{\dagger} \beta_{\mathbf{k}} + 1)$$

$$= E_{0} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} (\alpha_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \beta_{\mathbf{k}}^{\dagger} \beta_{\mathbf{k}}), \tag{44}$$

where we have defined

$$\omega_{\mathbf{k}} = JSz\sqrt{1 - \gamma_{\mathbf{k}}^2} \tag{45}$$

¹⁰We use that $\cosh^2 x + \sinh^2 x = \cosh 2x$ and $2 \cosh x \sinh x = \sinh 2x$.

and

$$E_0 = -NJS^2 z/2 - NJSz/2 + \sum_{\mathbf{k}} \omega_{\mathbf{k}}.$$
 (46)

Eq. (44) expresses the Hamiltonian in its final, diagonal form. The operators $\alpha_{\mathbf{k}}^{\dagger}$ and $\beta_{\mathbf{k}}^{\dagger}$ create magnon excitations with wavevector \mathbf{k} and energy $\omega_{\mathbf{k}}$. These magnons are bosons, and are noninteracting in the approximation used here (i.e. when only including terms of $O(S^2)$ and O(S) in the Hamiltonian). Note that in this antiferromagnetic case, for each \mathbf{k} there are two types of magnons (α and β) which are degenerate in energy. On the other hand, the \mathbf{k} sum goes over the magnetic Brillouin zone which only has N/2 \mathbf{k} vectors, so the total number of magnon modes is $2 \cdot N/2 = N$, the same as for the ferromagnetic case. Note that as $\mathbf{k} \to 0$, $\omega_{\mathbf{k}} \to 0$ as in the ferromagnetic case, but unlike the ferromagnetic case, for which a quadratic dispersion $\omega_{\mathbf{k}} \propto |\mathbf{k}|^2$ was found in this limit, in the antiferromagnetic case we have instead a linear dispersion,

$$\omega_{\mathbf{k}} \propto |\mathbf{k}| \text{ as } \mathbf{k} \to 0.$$
 (47)

In the ground state of \mathcal{H} (call it $|G\rangle$) there are neither α_k nor β_k magnons as these cost an energy $\omega_k > 0$. Thus $|G\rangle$ can be defined by the relations

$$\alpha_{\mathbf{k}}|G\rangle = 0, \quad \beta_{\mathbf{k}}|G\rangle = 0, \text{ for all } \mathbf{k}.$$
 (48)

This gives $\mathcal{H}|G\rangle = E_0|G\rangle$, i.e. the ground state energy is E_0 , given in Eq. (46). The first term $-NJS^2z/2$, i.e. the term $\propto S^2$, is just the ground state energy $E_{\rm class}$ of a classical nearest-neighbor antiferromagnet of spins with length S. The other terms are $\propto S$ and represent quantum corrections to the classical ground state energy. Note that this quantum correction ΔE is negative:

$$\Delta E = E_0 - E_{\text{class}} = \sum_{\mathbf{k}} \omega_{\mathbf{k}} - NJSz/2 = JSz \sum_{\mathbf{k}} \left[\sqrt{1 - \gamma_{\mathbf{k}}^2 - 1} \right]. \tag{49}$$

Thus quantum fluctuations lower the energy of the system. (Note that ΔE was 0 in the ferromagnetic case, i.e. there were no quantum fluctuations in the ferromagnetic ground state.)

Let us next investigate the amount of magnetic order in the system. Thus we need to identify an order parameter for antiferromagnetic order. Note that the magnetization $\mathbf{M} = (1/N) \sum_i \langle \mathbf{S}_i \rangle$ can not be used since it is zero in the presence of antiferromagnetic order, because the two sublattices give equal-magnitude but opposite-sign contributions to \mathbf{M} . Instead the natural order parameter is the so-called *sublattice magnetization*, defined by averaging $\langle \mathbf{S}_i \rangle$ only over the sites of one of the two sublattices. Without loss of generality, let's pick sublattice A, where the putative ordering is in the z direction. The magnitude of the sublattice magnetization is thus

$$M_A = \frac{1}{N_A} \sum_{j \in A} \langle S_j^z \rangle = S - \frac{1}{N_A} \sum_{j \in A} \langle a_j^{\dagger} a_j \rangle = S - \frac{1}{N_A} \sum_{\mathbf{k}} \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle. \tag{50}$$

Writing $M_A = S - \Delta M_A$, the correction ΔM_A to the classical result S is therefore given by

$$\Delta M_A = \frac{1}{N_A} \sum_{\mathbf{k}} \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle. \tag{51}$$

We need to rewrite this further in terms of the α and β type magnon operators, as it is in terms of them that the Hamiltonian takes its simple harmonic oscillator form. This gives

$$\Delta M_A = \frac{2}{N} \sum_{\mathbf{k}} \left[u_{\mathbf{k}}^2 \langle \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \rangle + v_{\mathbf{k}}^2 \langle \beta_{-\mathbf{k}} \beta_{-\mathbf{k}}^{\dagger} \rangle + u_{\mathbf{k}} v_{\mathbf{k}} \langle \alpha_{\mathbf{k}} \beta_{-\mathbf{k}} + \text{h.c.} \rangle \right].$$
 (52)

Now we can calculate the expectation values. They are both thermal and quantum, i.e. $\langle O \rangle \equiv Z^{-1} \sum_{m} \langle m | O | m \rangle e^{-\beta E_m}$ where $Z = \sum_{m} e^{-\beta E_m}$. Here the sum \sum_{m} is over the eigenstates $\{|m\rangle\}$ of \mathcal{H} with energy eigenvalues E_m and $\beta = 1/(k_B T)$ where T is the temperature and k_B is Boltzmann's constant. First consider

$$\langle \alpha_{\mathbf{k}} \beta_{-\mathbf{k}} \rangle = Z^{-1} \sum_{m} \langle m | \alpha_{\mathbf{k}} \beta_{-\mathbf{k}} | m \rangle e^{-\beta E_{m}}$$
(53)

and its complex conjugate. The summand involves $\langle m|\alpha_{\mathbf{k}}\beta_{-\mathbf{k}}|m\rangle$, which is the overlap of the states $\beta_{-\mathbf{k}}|m\rangle$ and $\alpha_{\mathbf{k}}^{\dagger}|m\rangle$. Both states are eigenstates of \mathcal{H} , but as they clearly do not have identical sets of occupation numbers of the various α and β bosons, their overlap is zero. Hence $\langle \alpha_{\mathbf{k}}\beta_{-\mathbf{k}}\rangle$ and its c.c. are zero. Thus

$$\Delta M_A = \frac{2}{N} \sum_{\mathbf{k}} \left[u_{\mathbf{k}}^2 \langle \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \rangle + v_{\mathbf{k}}^2 \langle \beta_{\mathbf{k}}^{\dagger} \beta_{\mathbf{k}} \rangle + v_{\mathbf{k}}^2 \right]$$

$$= \frac{2}{N} \sum_{\mathbf{k}} \left[n_{\mathbf{k}} \cosh 2\theta_{\mathbf{k}} + \frac{1}{2} (\cosh 2\theta_{\mathbf{k}} - 1) \right]$$

$$= -\frac{1}{2} + \frac{2}{N} \sum_{\mathbf{k}} \left(n_{\mathbf{k}} + \frac{1}{2} \right) \frac{1}{\sqrt{1 - \gamma_{\mathbf{k}}^2}}.$$

$$(54)$$

Here we used that $\langle \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \rangle = \langle \beta_{\mathbf{k}}^{\dagger} \beta_{\mathbf{k}} \rangle = 1/(e^{\beta \omega_{\mathbf{k}}} - 1) \equiv n_{\mathbf{k}}$ and $\cosh 2\theta_{\mathbf{k}} = 1/\sqrt{1 - \gamma_{\mathbf{k}}^2}$ (the last result follows from $\cosh^2 x = 1/(1 - \tanh^2 x)$).

We will not analyze Eq. (55) in its full glory, but briefly consider a few important points. This expression has a temperature-dependent part coming from n_k (note that $n_k = 0$ at T = 0) and a temperature-independent part coming from the two terms containing the factor 1/2. Let us first consider the case of zero temperature. In one dimension the k-sum becomes (note $\gamma_k = \cos k$ in one dimension)

$$\frac{1}{N} \sum_{k} \frac{1}{\sqrt{1 - \gamma_k^2}} \propto \lim_{k_0 \to 0} \int_{k_0}^{\pi/2} \frac{dk}{\sqrt{1 - \cos^2 k}}.$$
 (56)

The most important contribution to this integral comes from the small-k region where we can approximate $\cos k \approx 1 - k^2/2$. Thus the leading term becomes $\int_{k_0} dk/k = -\log k_0 \to \infty$ as $k_0 \to 0$. Thus ΔM_A diverges even at zero temperature. We must therefore conclude that for this one-dimensional case our assumption that the system was magnetically ordered is invalid and so is our truncated spin-wave expansion. Note that this conclusion holds for any S. In two dimensions at zero temperature ΔM_A is still nonzero so quantum fluctuations do reduce the magnetization, but the correction turns out to be small enough, $\Delta M \approx 0.2$, so that even for the lowest spin, S = 1/2, spin-wave theory indicates that the system is ordered

at zero temperature for a square lattice. This is also in agreement with other methods. In three dimensions ΔM is even smaller so the order is more robust then.

Next we consider finite nonzero temperatures. We just summarize the results that are obtained by analyzing (55) (which, we stress, is valid for a hypercubic lattice). In one dimension there is of course no antiferromagnetic order since none existed even at zero temperature. In two dimensions it turns out that the order does not survive at finite temperatures, so the spin-wave approach again is invalid. In three dimensions the system is ordered at sufficiently low temperatures.

5 Summary of spin-wave results

In the table below we summarize the main conclusions we have obtained from applying spin-wave theory to the Heisenberg ferromagnet and antiferromagnet on a hypercubic lattice in d spatial dimensions (d = 1, 2, 3). "Ordered" means spin-wave theory predicts magnetic ordering of the ferromagnetic/antiferromagnetic type, "disordered" means spin-wave theory predicts the absence of such order.

	Ferromagnet	Antiferromagnet
d = 1, T = 0	Ordered	Disordered
d = 1, T > 0	Disordered	Disordered
d = 2, T = 0	Ordered	Ordered
d = 2, T > 0	Disordered	Disordered
d = 3, T = 0	Ordered	Ordered
d = 3, T > 0	Ordered (at low T)	Ordered (at low T)

6 Broken symmetry and Goldstone modes

6.1 Broken symmetry

By definition, a symmetry transformation of a Hamiltonian is a transformation that leaves the Hamiltonian invariant. As an example, the Heisenberg Hamiltonian (1) considered in these notes is invariant under global spin rotations. Therefore we say that the Heisenberg Hamiltonian has a global spin rotation symmetry. A global spin rotation (\boldsymbol{w}, ϕ) is a transformation in which all the spin operators \boldsymbol{S}_i are rotated by the angle ϕ around the axis \boldsymbol{w} (more precisely, \boldsymbol{w} is a unit vector that points in the direction of the rotation axis). The word 'global' refers to the fact that all spin operators are rotated in the same way. The invariance of the Heisenberg Hamiltonian under global spin rotations can be understood intuitively by noting that if the spins had been just classical vectors, rotating them all in the same way preserves the angles between them and thus it also preserves the scalar products $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ in the Heisenberg Hamiltonian. The same conclusion can be shown to hold for the quantum case.¹¹

¹¹The rotations can be effected using *rotation operators*, which we haven't covered in this course. See e.g. Ch. 3 in J. J. Sakurai, "Modern quantum mechanics", revised edition, Addison-Wesley, 1994.

When the ground state of the Heisenberg Hamiltonian is magnetically ordered (either ferromagnetically for J < 0 or antiferromagnetically for J > 0), so that $\langle S_i \rangle \neq 0$, this ground state is **not** invariant under a global spin rotation. For example, if we have a ferromagnetically ordered ground state with all the spins pointing in the z direction, rotating this state by an angle ϕ around a general axis \boldsymbol{w} leads to a different ferromagnetically ordered ground state with all spins pointing in a different direction. As a concrete example, if we rotate all spins by 90 degrees around the negative x direction, after the rotation all the spins would point in the y direction. Clearly the nonzero order parameter \boldsymbol{M} is also not invariant; it undergoes exactly the same rotation as the spins. The same conclusion also holds for the antiferromagnetic ground state and its order parameter.

To describe this situation we say that the ground state "spontaneously" **breaks** the global spin rotation symmetry of the Hamiltonian. More generally, spontaneous¹² symmetry breaking refers to the situation when the ground state of the Hamiltonian is less symmetric than the Hamiltonian, i.e. the ground state is not invariant under all transformations that leave the Hamiltonian invariant.

For simplicity we focused on the ground state here. The notion of spontaneous symmetry breaking can however be generalized to systems at finite temperature: the equilibrium state of the Heisenberg model is said to exhibit spontaneous symmetry breaking if it has magnetic order, i.e. if its order parameter is nonzero. More generally, most known ordered phases of matter can be described in terms of broken symmetries.^{13,14}

6.2 Goldstone modes

Symmetries of a Hamiltonian can be classified as discrete or continuous. A symmetry is discrete if the associated symmetry transformations form a discrete set. In contrast, a symmetry is continuous if the associated symmetry transformations form a continuous set. The global spin-flip symmetry of an Ising model is an example of a discrete symmetry. The global spin-rotation symmetry of the Heisenberg model, on the other hand, is a continuous symmetry, since the rotations form a continuous set.

We found that both in the ferromagnetic and antiferromagnetic Heisenberg model, the magnon excitations have an energy ω_k that goes to zero as $k \to 0$. This implies that there is no gap in the excitation spectrum, i.e. there is no minimum nonzero energy cost to creating an excitation. We say that the magnon excitations are gapless. When the ground state of the Heisenberg model is magnetically ordered and thus breaks the continuous symmetry of the Heisenberg model, these gapless excitations are a consequence of the so-called Goldstone theorem, and are therefore also sometimes referred to as Goldstone modes or Goldstone bosons. The Goldstone theorem implies that when the ground state breaks a continuous symmetry of the Hamiltonian, gapless bosonic excitations will exist in the energy spectrum.

 $^{^{12}}$ To understand the meaning of the word "spontaneous" here, consider again the magnetically ordered ground state of the Heisenberg model. The ordering direction of the spins can be any direction; the actual ordering direction is chosen by the system "spontaneously".

¹³The fact that symmetries can be spontaneously broken is mathematically rather subtle. We haven't had time to go into that here; see e.g. the discussion in Ch. 2 in N. Goldenfeld, "Lectures on phase transitions and the renormalization group", Westview Press, 1992.

¹⁴Much research, both theoretical and experimental, is currently being done looking for novel phases of matter with more subtle types of order that cannot be described in terms of broken symmetries.

¹⁵More precisely, a generalized version of this theorem due to Nielsen and Chadha.