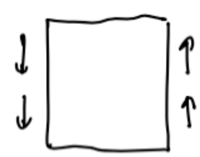
Oct. 24

Physics 212 – Statistical Mechanics

Broken Symmetry, Topology, and Classical Solutions

In the previous lecture, I discussed the possible ground states of a Statistical Mechanical system with spontaneously broken symmetry. I explained how to use Landau theory to find the possible thermodynamic states and to compute correlation functions. This gave a local description of each individual ground state. In this lecture, I would like to broaden the discussion to analyze features of the space of broken-symmetry states.

Let's first discuss the Ising case, in the region $T < T_c$. Here we have a discrete set of 2 ground states of the free energy. Each of these has a uniform expectation value of the magnetization. But this raises the following question: If we choose boundary conditions such that the spins are required to up down as $x \to -\infty$ but up as $x \to +\infty$, what is the resulting state?



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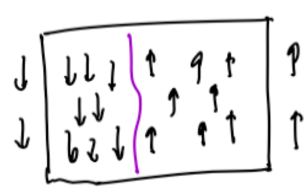
Think about filling in the configuration of spins smoothly from each boundary. In most of the interior, we will be in one ground state or the other. However, at some value of x, there must be a transition – a *domain wall*.



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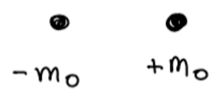
This transition must cost free energy. How can we describe it?

I will show you that Landau theory gives us a description of the domain wall. This is an example of a general phenomenon. If a thermodynamics system has multiple stable states, it is possible to find a configuration that approaches different ones of these states as we go to infinity in different directions. This configuration will be nontrivial in the interior of the system, and it will have positive free energy above the free energy of the ground states. However, it is possible that this configuration will be a local minimum of the free energy, and that it will be unable to dissipate its free energy while the magnetization field remains continuous. This can occur due to the topolgy of the manifold of ground states. We then have a *topologically stable solution* of the thermodynamic equations.

This situation applies to the domain wall. Let me now show this explicitly. This description will seem like overkill for the example of the domain wall, but it has nontrivial generalizations.

In the Ising model at low temperatures, the space of ground states is discrete,



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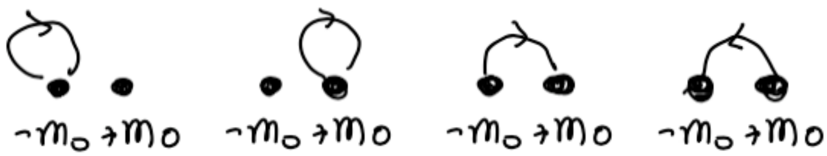
As we go to infinity in any direction, the system should be in one of these ground states. However, if we consider continuous configurations that depend on the coordinate x, there are four possibilities,



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These form different topological classes. In the first two cases, the system can relax to a uniform state. In the second two cases, there is no continuous deformation of the configuration that can bring it into one of the earlier classes. In each of these sectors, there is a solution with lowest free energy. That solution is *topologically stable*. It has excess free energy above the ground state, but this free energy cannot be released.

Toward the end of the lecture, and in the following lectures, I will discuss additional examples of this phenomenon in models with $SO(2)$ and $SO(n)$ symmetry.

What is the exact form of the domain wall in the Ising model? This question is difficult to address in general, but, near $T = T_c$, we can use Landau theory to find the answer. We start from the variational equation for the magnetization $m(\vec{x})$,

$$-\nabla^2 - a(T_c - T)m + bm^3 = 0 \tag{5}$$

We seek a solution to this equation of the form of a function of one dimension x

$$m(x) \qquad \text{independent of } y,\ z \tag{6}$$

with the boundary conditions

$$m(x) \to -m_0 \text{ as } x \to -\infty\ , \quad m(x) \to +m_0 \text{ as } x \to +\infty \tag{7}$$

There is a general method for finding such solutions qualitatively. Temporarily replace the variable x by t and consider $m(t)$ to be the position of a particle. Then we can interpret the variational equation as the equation of the motion of this particle in a potential. Writing this equation as

$$\frac{d^2}{dt^2}m = -a(T_c - T)m + bm^3 \tag{8}$$

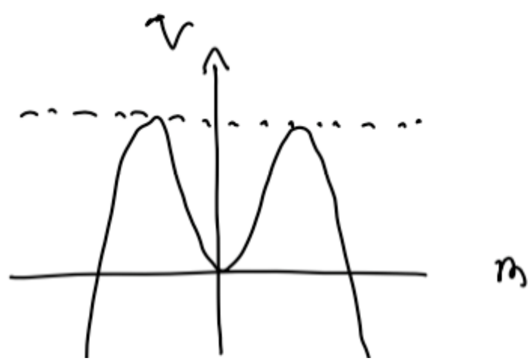
we can recast this as

$$\frac{d^2}{dt^2}m = -\frac{\partial}{\partial m}V(m) \ , \tag{9}$$

and think of the function $V(m)$ as a potential energy. Here, the potential $V(m)$ is the reverse of the potential in the Gibbs free energy,

$$V(m) = +\frac{1}{2}a(T_c - T)m^2 - \frac{1}{4}bm^4 \tag{10}$$

and so has the form



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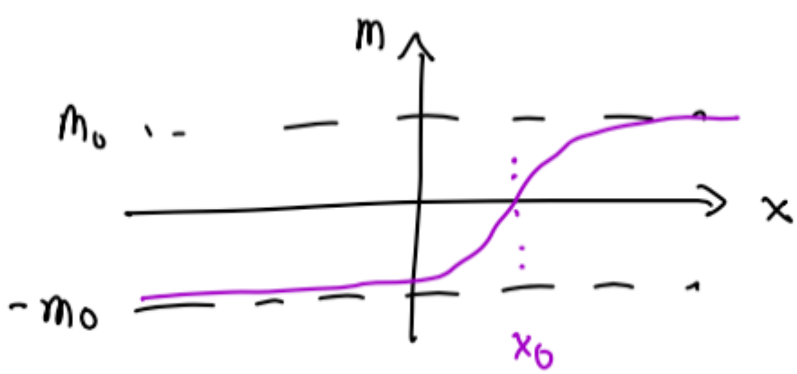
The solution that we are seeking is the motion that starts with zero kinetic energy at the peak on the left, rolls down into the valley, and asymptotically comes to rest at the top of the peak on the right. Then,



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The crossover is not attached to any particular time t. So actually, we have a family of solutions. Going back from t to x, we have a solution with the crossover at any position x_0,

$$m(x - x_0)\ . \tag{13}$$

There is no energy difference between the solutions with the domain wall at different positions (as long as the position x_0 is not near one of the boundaries). Each solution breaks the translation invariance in x.

Actually, for this particular differential equation, there is a simple analytic solution. Using

$$m_0^2 = \frac{a(Tc - T)}{b} \tag{14}$$

we can write the equation as

$$\frac{1}{a(T_c - T)}\frac{d^2}{dx^2}m = -(1 - \frac{m^2}{m_0^2})\ m\ . \tag{15}$$

Let

$$z = \frac{x}{2}[2a(T_c - T)]^{1/2} = \frac{x}{2\bar{\xi}}\ , \tag{16}$$

noting that the correlation length in the magnetized phase is

$$\bar{\xi} = 1/[2a(T_c - T)]^{1/2}\ . \tag{17}$$

Then the equation becomes

$$\frac{1}{2}\frac{d^2}{dz^2}\frac{m}{m_0} = -(1 - \frac{m^2}{m_0^2})\ \frac{m}{m_0}\ . \tag{18}$$

A solution is

$$m(z) = \tanh z \tag{19}$$

To check this, note that

$$\frac{d^2}{dz^2}\tanh z = \frac{d}{dz}\frac{1}{\cosh^2 z} = -2\frac{\sinh z}{\cosh^3 z} = -2\frac{1}{\cosh^2 z}\tanh z\ . \tag{20}$$

The general solution of the equation that remains regular when $x \to \pm\infty$ is then

$$m(x) = m_0\ \tanh\left(\frac{x - x_0}{2\bar{\xi}(t)}\right) \tag{21}$$

Note that, as $x \to \infty$, this solution approaches the asymptotic uniform state as

$$m(x) \sim m_0\left(1 - 2e^{-(x-x_0)/\bar{\xi}(T)}\right)\ , \tag{22}$$

in accord with the definition of the correlation length.

The excess free energy associated with the domain wall is

$$\Delta G = \int d^3x \Big(\frac{1}{2}(\vec{\nabla} m)^2 - \frac{1}{2} a(T_c - T) m^2 + \frac{1}{4} m^4 - (-\frac{b}{4} m_0^4) \Big) \ . \tag{23}$$

Subsituting again $z = x/2\overline{\xi}$, with

$$a(T_c - T) = \frac{1}{2\overline{\xi}^2} \qquad b = \frac{b}{a(T_c - T)} \frac{2a(T_c - T)}{2} = \frac{1}{2\overline{\xi}^2 m_0^2} \ , \tag{24}$$

this expression becomes

$$\begin{aligned} \Delta G &= \mathcal{A} \int_{-\infty}^{\infty} dx \Big\{ \frac{1}{8\overline{\xi}^2} (\frac{dm}{dz})^2 - \frac{m^2}{4\overline{\xi}^2} + \frac{1}{8\overline{\xi}^2} \frac{m^4}{m_0^4} + \frac{m_0^2}{8\overline{\xi}^2} \Big\} \\ &= \mathcal{A} \, \frac{m_0^2}{8\overline{\xi}^2} \cdot 2\overline{\xi} \cdot \int_{-\infty}^{\infty} dz \, \Big\{ (\frac{1}{\cosh^2 z})^2 + (1 - \tanh^2 z)^2 - 1 + 1 \Big\} \ , \end{aligned} \tag{25}$$

where $\mathcal{A}$ is the area of the domain wall. Then we find

$$\Delta G = \mathcal{A} \cdot \frac{m_0^2}{4\overline{\xi}} \int_{-\infty}^{\infty} dz \, \frac{2}{\cosh^4 z} \ , \tag{26}$$

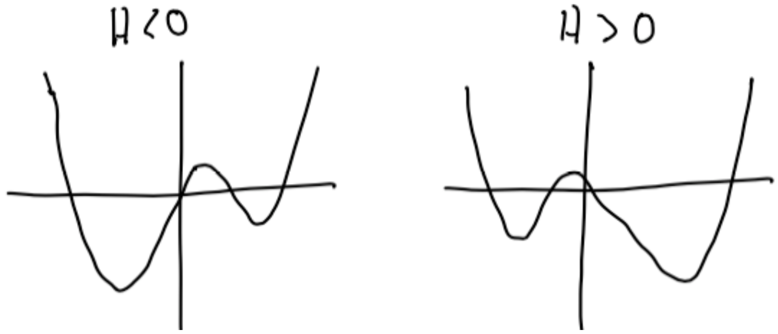
or

$$\Delta G = \mathcal{A} \cdot \frac{2}{3} \frac{m_0^2}{\overline{\xi}} \ . \tag{27}$$

The dependence on the parameters is the one we expect from dimensional analysis. The domain wall is a surface in 3-dimensional space; thus, the excess free energy ΔG is proportional to the area of this surface. If N is the number of atoms in the original model, this dependence is $N^{2/3}$, subdominant to the overall free energy. As $T \to T_c$, the *wall tension*, the free energy per unit area, vanishes as $(T_c - T)^{3/2}$. The functional form of the interface applies in the vicinity of $T = T_c$ in any ordered system that is that is described by the Landau theory for the Ising model, including the liquid-gas and binary liquid interfaces.

There is another interesting problem to which this formalism can be applied. If we have a discontinuous (first-order) phase transition, we can pass continuously across the transition line into a metastable phase. The most frequent application of this idea is to the liquid-gas phase transition, where it is called supercooling or superheating. For example, we can heat a sample of fluid above its boiling point. How does it make the transition to the gas phase? Here I will discuss the analogous transition in a magnet, where the Z_2 symmetry can help us a little.

Consider, then, a situation at $T < T_c$ in whch we prepare an Ising magnet in a small *negative* magnetic field and then reverse the field direction suddenly, changing the field to a *positive* value. The Gibbs free energies for the initial and final situations are



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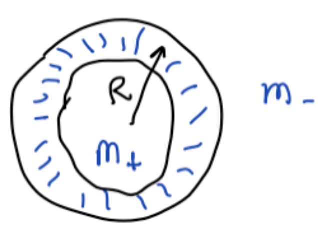
If the system evolves continuously, it moves from a globally stable ground state to a locally stable but globally unstable ground state. What happens next?

Since the state m_- is locally stable, the transition from m_- to m_+ requires crossing a free energy barrier. This can happen by a thermal fluctuation, but there is an *activation free energy* ΔG, corresponding to the minimal height of the barrier. The thermal fluctuation will be local, forming a small bubble of the favored phase. This bubble will then expand and, evenually, eat up the whole volume. The rate of the transition is then described by a rate of bubble formation per unit volume,

$$\Gamma \sim \frac{\text{rate}}{\text{volume}} \sim e^{-\beta \Delta G} \ . \tag{29}$$

Note that ΔG should be a local quantity, independent of the volume of the whole system.

To compute ΔG, we have to decide what is the size of the bubbles that will nucleate the transition. Let's first study this problem in a qualitative picture: The bubble is a configuration of $m(x)$ the goes to the ground state m_- at large radii but has a value close to m_+ at small values of the radius



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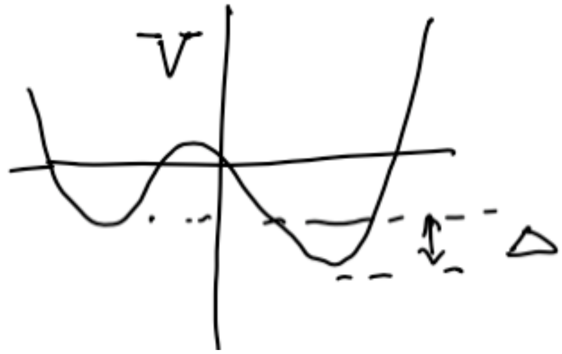
To estimate the free energy of such a bubble, let the free energy density gain from

m_- to m_+ be Δ,



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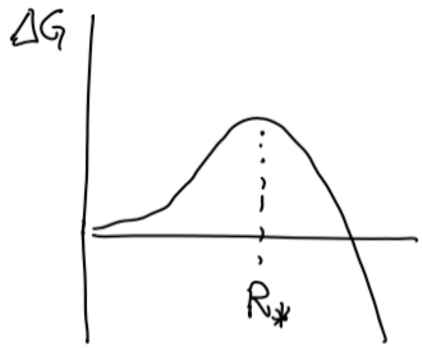
and let the wall tension of the domain wall separating the two possible locally stable states be τ. Then the excess free energy of the bubble is estimated as

$$\Delta G = +4\pi R^2 \tau - \frac{4}{3}\pi R^3 \Delta \ , \tag{32}$$

where R is the radius of the bubble. You can see that there is a competition between the free energy of the interior, which favors large bubbles, and the wall tension, which favors small bubbles. The overall function has the form



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with a maximum at a radius R_*, called the radius of the *critical bubble*. Maximizing our approximate equation, we find

$$8\pi R\tau = 4\pi R^2 \Delta \tag{34}$$

or

$$R_* = \frac{2\pi}{\Delta} \qquad \Delta G(R_*) = \frac{16\pi}{3}\frac{\tau^3}{\Delta^2} \ . \tag{35}$$

Since

$$\Delta = \eta (T_c - T)^{1/2} H \quad \text{and} \quad \tau = \zeta (T_c - T)^{3/2} \tag{36}$$

the bubble nucleation rate dependents on temperature and the magnetic field H as

$$\Gamma \sim \exp\Big[-\frac{16\pi}{3}\frac{\zeta^3}{\eta^2}\frac{(T_c - T)^{7/2}}{H^2}\Big] \ . \tag{37}$$

When a fluctuation of the size of the critical bubble occurs, this bubble expands to eventually convert the whole volume to the globally stable phase.

This is a somewhat crude theory, good for estimation only. We can find a more precise description of the critical bubble using Landau theory. The critical bubble should be a *maximum* of the free energy in the direction of R and a *mimimum* in all other directions. Thus, it will be an extremum of the free energy and therefore a solution to the variational equation

$$-\nabla^2 m - a(T_c - T)m + bm^3 - H = 0 \tag{38}$$

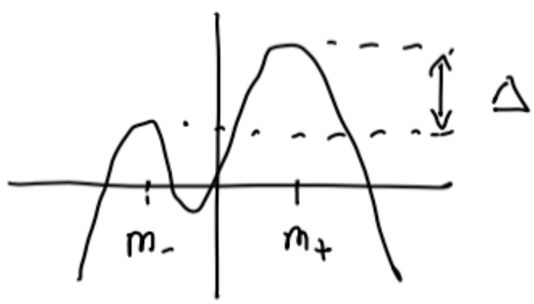
Let's look for a spherically symmetric solution to this equation. Recall that, in the 3 dimensions, acting on functions of r

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \tag{39}$$

Replacing r by the variable t, we find the equation

$$\frac{d^2}{dt^2} = -\frac{d}{dm}V(m) - \frac{2}{t}\frac{d}{dt}m \ , \tag{40}$$

where $V[m]$ is the reversed potential



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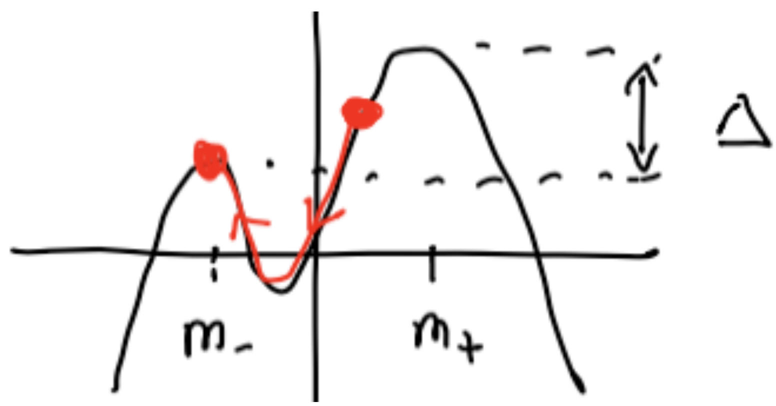
We are looking for a solution $m(t)$ that tends as $t \to \infty$ to the constant value m_-. The second term on the right-hand side of (40) is a friction term proportional to $1/t$. Then we should look for a solution that starts on the hill to the right, falls down into the valley, and ends up exactly on the top of the hill to the left with zero kinetic energy. Since there is dissipation, the initial value at $t = 0$ should be at a somewhat higher potentially energy than that of m_-. However, it cannot start at the top of the hills, since then there would not be enough dissipation to keep it from overshooting.

The form of the solution is then



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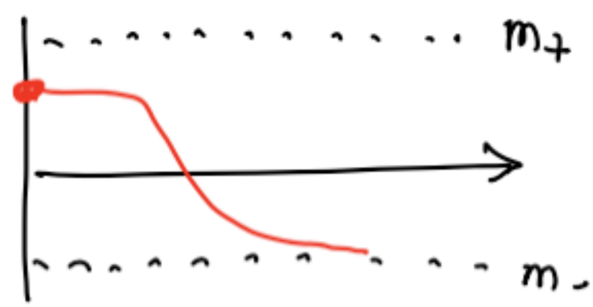
or, as a function of r,



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For those who enjoy such things, there is an analytic solution in terms of elliptic functions. As in the previous example, the shape of the bubble and its dependence on T and H will be the same in the region near $T = T_c$ for any system described by the Landau theory of the Ising model.

In the models with higher symmetry, the topology of the thermodynamic ground states changes. In the cases of $SO(2)$ and $SO(3)$ symmetry, the ground states are not isolated but rather form a continuous manifold. We should then look back at the problem of a magnetized state with boundary conditions of spin down as $x \to -\infty$ and spin up as $x \to +\infty$. The domain wall solution found above is still a solution to the Landau equations, but now there is a better solution.

Let's study first the case of the XY model with $SO(2)$ symmetry. The ground states form a manifold with the topology of a circle,

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The domain wall solution that we found for the Ising case is now a maximum of the Gibbs free energy,

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we can lower the energy by pushing the solution down onto the space of minima of $G[\vec{m}]$. Let me consider a system that is finite in x, with the boundary condition that

$$\vec{m}(x) \to -m_0\hat{x} \text{ as } x \to -L \ , \quad \vec{m}(x) \to +m_0\hat{x} \text{ as } x \to +L \tag{46}$$

For this situation, an easy path that satisfies the boundary conditions is

$$\vec{m}(x) = m_0(\sin\frac{\pi x}{2L}, \cos\frac{\pi x}{2L}) \tag{47}$$

The excess free energy of this state is

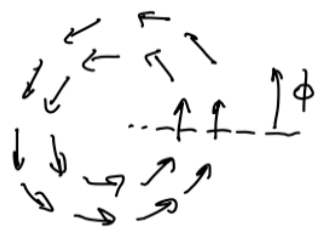
$$\begin{aligned} \Delta G &= \int d^3x \Big\{ \frac{1}{2}(\nabla^i \vec{m})^2 + 0 \Big\} \\ &= \mathcal{A}\int_{-L}^{L} dx \frac{\pi^2}{8L^2} m_0^2 \\ &= \mathcal{A} \cdot \frac{\pi^2}{4}\frac{m_0^2}{L} \ . \end{aligned} \tag{48}$$

In the limit of a large system $L \to \infty$, this excess free energy goes to zero! So there is no domain wall and no excess free energy. This solution is also available for the Heisenberg model and for any system with $SO(n)$ symmetry, $n \geq 2$.

On the other hand, the XY model has a different kind of localized solution in which $\vec{m}(x)$ has a different value at each angle as $r \to \infty$. An example is the configuration

$$\vec{m} = m_0(-\sin\phi, \cos\phi) \tag{49}$$

which we might call a “vortex”.



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This solution obeys

$$-\nabla^2 m^1 = \left(-\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} - \frac{1}{r^2}\frac{\partial}{\partial\phi}\right)(-m_0 \sin\phi)$$
$$= \frac{1}{r^2}(-m_0 \sin\phi) \tag{51}$$

This goes to 0 as $r \to \infty$, so we can find a solution of the form

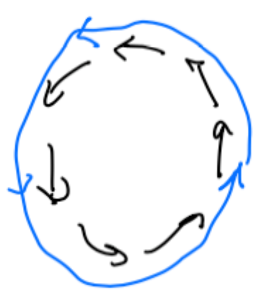
$$m(\vec{r}) = M(r)(-\sin\phi, \cos\phi) \tag{52}$$

where $M(r) \to m_0$ as $r \to \infty$. The excess free energy is

$$\Delta G = \int d^3x \frac{1}{2}(\nabla^i \vec{m})^2$$
$$= (\mathcal{L}) \cdot \int_0^\infty dr\ 2\pi r \left(\frac{m_0^2}{r^2}\right) \tag{53}$$

This is formally divergent as $r \to 0$, but in a realistic situation the integral would be cut off at the length scale of the atomic spacing.

The vortex solution cannot be continuously deformed to the ground state configuration. This is because its boundary condition at infinity is wrapped onto the manifold of vacuum states in a nontrivial way.



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This is another example of a topologically stable configuration. There are vortex solutions for any number of wrappings, that is, for any n with

$$\oint d\vec{x} \cdot \vec{m} = 2\pi n\ m_0 \tag{55}$$

However, that stability of these solutions depends on the specific situation of the XY model. For the Heisenberg model, the manifold of ground states has the topology of a sphere

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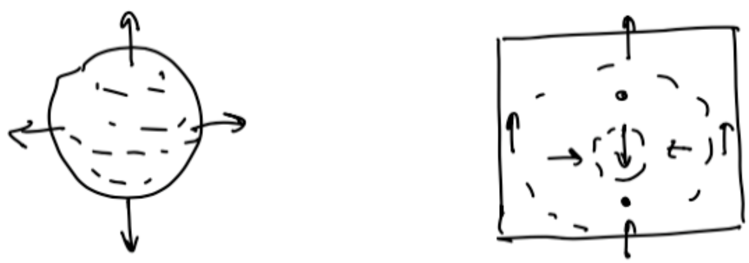
Now it is possible to continuously deform the boundary condition at infinity to the trivial configuration. Then the stability of the vortex solution is lost.

For each Landau theory, we will find in general a different form of the manifold of ground states. Each possibility offers a different set of topologically stable solutions. For $n = 3$ in 2 dimensions, there is a solution called the Skyrmion in which the manifold of ground states, which has the topology of a 2-dimensional sphere, is mapped in a topologically nontrivial way onto the 2-dimensional plane.



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The solution has positive energy from the gradient term in the Landau free energy, but it is possible to add a 4-derivative term that balances this contribution and stabilizes the radius of the solution at a finite value. Appropriate parameters are realized in some magnetic systems. Recently, these magnetic Skyrmions have been investigated for application to magnetic information storage. The Skyrme solution was originally introduced in 1962 by Tony Skyrme in its realization in the 3-dimensional $SO(4)$-symmetric theory, as a model of the structure of the proton. (Yes, the Landau theory of QCD, the theory of the strong interactions, is that of a magnetic model with $n = 4$.)

When an ordered system is created in a small system where the boundary conditions are important, more varied configurations, called "textures", can appear. These are of interest in liquid crystals and in superfluid He^3. For an example in the latter context, called the "boojum", see David Mermin's article Physics Today, 34, 41 (1981).