1 Lecture 1. Long-range order, symmetry and soft modes

1.1 Long-range order

The notion of *long-range order* is used to describe the situation when the state of a macroscopic system has symmetry lower than that of the system Hamiltonian. A system with a long range order is described by a symmetry group that transforms one state to another equivalent state. Two different situations are possible regarding this symmetry group: it can be (i) discrete or (ii) continuous.

A slightly artificial but very useful example of a discrete symmetry is an Ising magnet model. The variables are spins on a lattice, described by $\sigma_r = \pm 1$. The Hamiltonian of spin interaction is

$$\mathcal{H} = -\frac{1}{2}\sum_{r} J(r-r')\sigma_r\sigma_{r'} \tag{1}$$

where $J(r-r') > 0$ is exchange interaction. By convention, each pair of points r, r' is counted twice in the sum, which accounts for the factor $\frac{1}{2}$. At zero temperature, there are two lowest energy states: ALL spins up, $\sigma_r = +1$, or ALL spins down, $\sigma_r = -1$.

Note that the overall sign change $\sigma_r \to -\sigma_r$ leaves the Hamiltonian invariant, while the two ground states are not invariant. Under a sign change they transform into each other. In the group theory terminology, the symmetry group of the manifold of (in this case, just two) states is Z_2, consisting of the identity and the sign reversal transformations.

Such a situation is sometimes called *spontaneous symmetry breaking*. Indeed, think of someone presented with a choice of choosing a ground state. This choice is perfectly symmetric, since each of the possible ground states is equivalent to other states. However, as soon as the choice is made, the situation becomes asymmetric, because the state symmetry is lower than that of the Hamiltonian. This concept, especially in the cases when the symmetry group of possible ground states is continuous, has many applications in the high energy physics, cosmology, hydrodynamics, nonlinear dynamics and, of course, in condensed matter physics. We hope to explore this a bit more later, in homeworks, course-related projects or term papers.

1.2 Soft modes, general theory

In the situation when the symmetry group of different equivalent states is continuous, **Goldstone theorem** predicts that there exist soft modes, i.e. one or several branches of excitations with the energy vanishing in the limit of long wavelength.

Consider an example from field theory: an n–component field ϕ_i, $i = 1, ..., n$, with the Hamiltonian

$$\mathcal{H} = \int \left(\frac{1}{2}\pi_i^2 + \frac{1}{2}(\nabla\phi_i)^2 + U(|\phi|) \right) d^3x \tag{2}$$

Here the potential energy $U(|\phi|)$ depends only on the vector ϕ_i length, but not on its orientation. The first term in Eq.(2) is kinetic energy written in terms of momentum density π_i of the field ϕ_i.

When the potential energy $U(|\phi|)$ has a minimum at finite ϕ_0, there are infinitely many ground states, all with the same energy. They are described by constant field $|\phi(x)| = \phi_0$ with restricted length, but unrestricted direction. They manifold of ground states in this case is an $n-1$ dimensional sphere.

Perturb near one of these states. The state $\phi_i(x)$ slowly varying in space have energy which is larger but can be made arbitrarily close to the ground state energy by choosing sufficiently large wavelength.

Graphically, for a two component field, $n = 2$, the 3D plot U vs ϕ looks like a Mexican hat, with the manifold of ground states being a circle near the hat rim. If the field ϕ orientation is slowly varying in space, with the length $|\phi|$ fixed, it costs almost no energy.

More quantitative estimate: for $\phi_i(x) = \phi_i^{(0)} + \delta\phi_i(x)$ with the *transverse* pertubation $\delta\phi_i(x) = A_i \cos \mathbf{k}\cdot\mathbf{x}$ such that $A_i\phi_i^{(0)} = 0$, the energy density

$$\delta\mathcal{H} = \int (\nabla\delta\phi_i(x))^2 d^3x \propto \mathbf{k}^2 A^2 \tag{3}$$

Indeed, $\delta U \to 0$ when $k \to 0$.

Excitations are described by the Hamilton equations of motion:

$$\dot{\pi}_i = -\delta\mathcal{H}/\delta\phi_i = \nabla^2\phi_i - \partial U/\partial\phi_i\,, \quad \dot{\phi}_i = \delta\mathcal{H}/\delta\pi_i = \pi_i \tag{4}$$

Linearizing them for the excitations of small amplitude $|\delta\phi| \ll |\phi^{(0)}|$, obtain a wave equation $(\partial_t^2 - \nabla^2)\delta\phi_i = 0$, which gives a linear dispersion relation $\omega(k) = k$.

Alternatively, one can start with the Lagrangean

$$\mathcal{L} = \int \left(\frac{1}{2}\dot{\phi}_i^2 - \frac{1}{2}(\nabla\phi_i)^2 - U(|\phi|) \right) d^3x\,. \tag{5}$$

Linearizing $\mathcal{L}(\phi)$ in small perturbation amplitude $\delta\phi$, obtain

$$\mathcal{L} = \int \left(\frac{1}{2}(\delta\dot{\phi}_i)^2 - \frac{1}{2}(\nabla\delta\phi_i)^2) \right) d^3x \tag{6}$$

which yields the same wave equation.

The mode with a "soft" dispersion relation, such that $\omega(k) \to 0$ when $k \to 0$, is called *a Goldstone mode*. To summarize the discussion of the example (2), spontaneous symmetry breaking with a continuous group of ground state transformations (described also as continuous order parameter degeneracy), gives rise to *Goldstone modes* with soft dispersion relation.

It will be crucial for us that the statistical properties of such a system at low enough temperature are *entirely determined* by these low energy excitations. They are the thermodynamically active degrees of freedom that describe thermal energy excitations and thermodynamic fluctuations in equilibrium. Typically, by analyzing the system and characterizing the low energy excitations (soft modes), one can reduce a relatively complicated problem to a much simpler problem. Moreover, the initial microscopic problem is usually case-sensitive, while the problem obtained by isolating the low energy modes is usually more universal, with the basic features determined only by symmetry (and perhaps by several "material constants").

Comment 1: A problem very similar to Eq.(2), with $n = 2$ and $U(\phi) = \frac{1}{2}g(\phi^2 - n)^2$, describes a superfluid (see Problem 1 in PS#1). The wavefunction ψ in this homework problem is complex-valued. Writing it as $\psi = \phi_1 + i\phi_2$, see that the only difference is the form of kinetic energy: $\frac{1}{2}\dot{\phi}_i^2 \to i\bar{\psi}\partial_t\psi+$c.c.. The conclusions about low energy excitations, however, are unchanged.

Comment 2: To see why is it so important for the Goldstone theorem to have a continuous manifold of degenerate states, consider the form of the energy $U(\phi) = \frac{1}{2}U_0\phi^2$ with a single minimum at $\phi = 0$. Then the ground state is $\phi = 0$. Pertubing about it, obtain an equation with a mass term, $(\partial_t^2 - \nabla^2 + U_0)\delta\phi_i = 0$, which gives a dispersion relation with a cutoff frequency: $\omega(k) = (k^2 + U_0)^{1/2}$. No low energy excitations in this case.

1.3 Different systems, often the same symmetry classes

Now let us consider several other examples of interest for statistical mechanics. To illustrate the generality of the relation between continuous symmetry and soft modes, we shall consider seemingly distant systems: solid, liquid crystal, ferromagnet, incommensurate crystal.

Elastic modes in solids are described by displacements of atoms in a crystal lattice relative to equilibrium positions. The hamiltonian of atoms and nuclei is invariant under spatial translations and Euclidean rotations. The crystal itself, however, is not invariant, since translating it by a constant vector incommensurate with lattice period gives a geometrically different but physically equivalent crystal. Similarly, spatial rotation changes the crystal to a different crystal.

The soft modes of a crystal are described by displacement fields slowly varying in space. Indeed, constant displacement field correponds to an overall translation by a constant vector, and thus does not change energy. Weakly nonuniform translation will change energy, but thsi change will be small when the wavelength of spatial modulation is large. The long wavelength displacements are thus *the Goldstone modes* in this case.

The Hamiltonian of elastic modes in a crystal is written in terms of gradients of the displacement field $u_i(x)$ as[1]

$$E(u) = \int \left(\frac{\lambda}{2} u_{ii}^2 + \mu u_{ij}^2 \right) d^3x \tag{7}$$

with $u_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$ the deformation tensor and Lame constants λ, μ.

We stress that the form of the elastic energy can be deduced solely from a symmetry argument. Indeed, the energy $E(u)$ cannot depend on u_i, but only on its gradients $\partial_i u_j$, since an explicit dependence on u renders the energy noninvariant under uniform spatial translations $u_i(x) \to u_i(x) + a_i$, where $\mathbf{a}$ is a constant vector. Furthermore, to the lowest order in gradients, the energy has to be quadratic in the tensor $\partial_i u_j$. One might expect that, since there are $3 \times 3 = 9$ different components in $\partial_i u_j$, the energy dependence on the displacement field will be complicated. Remarkably, this is not the case. The condition of rotational symmetry leaves one with three invariants $\partial_i u_j \partial_i u_j$, $\partial_i u_j \partial_j u_i$ and $\partial_i u_i \partial_j u_j$. However, there is no dependence of the energy on the the antisymmetric part $\partial_i u_j - \partial_j u_i$ of the tensor $\partial_i u_j$, since it describes an infinitesimal rotation which does not change system energy. Thus there are only two independent terms in the elastic energy (7).

The kinetic energy is $\int \frac{1}{2}\rho \dot{u}_i^2 d^3x$ with ρ the crystal density. The dynamics is described by the Lagrangean $\mathcal{L} = \int \left(\frac{1}{2}\rho \dot{u}_i^2 - \frac{\lambda}{2} u_{ii}^2 - \mu u_{ij}^2\right) d^3x$, or (same thing!) by Newton's equations

$$\rho \ddot{u}_i = \delta E(u)/\delta u_i \tag{8}$$

One can look for a plane wave solution $u_j(x) = u_j e^{i\mathbf{k}\cdot\mathbf{x} - i\omega t}$, which gives three coupled linear equations for the vibration amplitude

$$\omega^2 u_i = \lambda k_i k_j u_j + \mu k_j \left(k_i u_j + k_j u_i\right) \tag{9}$$

There are three normal modes, one longitudinal with $\mathbf{u} \parallel \mathbf{k}$ and two transverse, with $\mathbf{u} \perp \mathbf{k}$. All three have linear dispersion $\omega \propto k$. the velocities of the longitudianl and transverse sound are different. For the longitudinal mode, $\omega(k) = c_l k$ with the velocity $c_l = \sqrt{(\lambda + 2\mu)/\rho}$. For the transverse mode, $\omega(k) = c_t k$ with $c_l = \sqrt{\mu/\rho}$.

Thermal excitation of long wavelength vibrational modes controls thermodynamical properties of this system. The elementary excitations associated with the vibrational modes, also called phonons, are Bose particles. The occupation number of a mode with wavevector k is given by Planck distribution: $n_k = 1/(e^{\beta\omega(k)} - 1)$ with $\beta = 1/T$. This means that only modes with sufficiently long wavelength,

$$\omega(k) = c_{l,t}(2\pi/\lambda) \le T \tag{10}$$

are thermally excited[2].

The thermodynamic potential of this system is

$$\Omega = T \int \ln(1 - e^{-\omega_l(k)/T}) \frac{d^3k}{(2\pi)^3} + 2T \int \ln(1 - e^{-\omega_t(k)/T}) \frac{d^3k}{(2\pi)^3} \tag{11}$$

[1] This simple form of elastic energy is correct for an isotropic solid, such as a glass or a polycrystal. In a real crystal, elastic energy has more complicated form: $E(u) = \frac{1}{2}\int \lambda_{ijkl} u_{ij} u_{kl} d^3x$ with λ_{ijkl} an anisotropic elasticity tensor.

[2] Unless stated otherwise, we use absolute temperature units with the Boltzmann constant $k_{\mathrm{B}} = 1$.

Here the integral over k adds up the contributions of modes with different wavelengths, while the factor 2 accounts for two transverse modes. This expression can be used to obtain the entropy, specific heat, and other thermodynamic quantities.

Liquid crystal

There is a strange state of matter intermediate between liquids and solids, called liquid crystals. These are fluids with one or another form of orientational order. Microscopically, they consist of relatively large anisotropic molecules, such as long rods, which have orientations correlated with each other throughout the entire volume of the liquid crystal. For a more detailed but still quite general discussion of a nematic state we refer to a very good book "Physics of liquid crystals," by de Gennes.

there are many interesting phases of liquid crystals. In the simplest case of a nematic ordering, the system is translationally invariant, while the rotational invariance is broken. Average molecule direction is described by a "director" vector $\pm\mathbf{n}$. The order parameter is a symmetric traceless tensor $Q_{ij} = Q(T)(n_i n_j - \frac{1}{3}\delta_{ij})$.

The system has rotational degeneracy described by all possible orientations of $\mathbf{n}$, – a 2D sphere with opposite points identified (a projective plane, in topolgical terms). Thus the energy cannot depend on $\mathbf{n}$ only. The dependence on the gradients $partial_i n_j$ can be deduced from the rotational invariance of the problem.

The logic is similar to that used above in the discussion of elasticity. The energy of a liquid crystal in a uniform state with constant $\mathbf{n}$ does not depend on the orientation of $\mathbf{n}$ (the ground state degeneracy). Hence the energy has to depend on the gradients $\nabla\mathbf{n}$.

(i) $E(\mathbf{n})$ must be even in $\mathbf{n}$, as explained above, the states $(\mathbf{n})$ and $(-\mathbf{n})$ are undistinguishable;

(ii) No terms linear in $\mathbf{n}$. The only terms of this form invariant under rotation are $\operatorname{div}\mathbf{n}$ (ruled out by (i)) and $\mathbf{n}\cdot\operatorname{curl}\mathbf{n}$ (changes sign by the transformation $(x, y, z) \to (-x, -y, -z)$);

Thus $E(\mathbf{n})$ should be quadratic in ∇. The simples way to list all possible rotationally invariant terms of this form is to consider three quatities,

$$\operatorname{div}\mathbf{n}, \quad \mathbf{n}\cdot\operatorname{curl}\mathbf{n}, \quad \mathbf{n}\times\operatorname{curl}\mathbf{n}, \tag{12}$$

and take a sum of squares. One can show (this is tedious but elementary[3]) that this accounts for all possible terms of second order in gradients. Thus the elastic energy of a liquid crystal is

$$E(\mathbf{n}) = \frac{1}{2}\int \Big(\mathcal{K}_1(\operatorname{div}\mathbf{n})^2 + \mathcal{K}_2(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 + \mathcal{K}_3(\mathbf{n}\times\operatorname{curl}\mathbf{n})^2\Big)\, d^3x \tag{13}$$

The constants $\mathcal{K}_{1,2,3}$ account for the energy cost of conformations with nonzero $\operatorname{div}\mathbf{n}$, $\mathbf{n}\cdot\operatorname{curl}\mathbf{n}$ and $\mathbf{n}\times\operatorname{curl}\mathbf{n}$. They are known as the splay, twist and bend modulus, respectively.

The dynamics is of relaxational form: $\dot{\mathbf{n}} = -\gamma\delta E(\mathbf{n})/\delta\mathbf{n}$. Two relaxational soft modes with complex disperion relation $\omega \propto ik^2$.

Thermal excitations are fully described by the elastic energy (13). To analyze thermal excitations, one can consider a weakly modulated state, $\mathbf{n}(x) = \mathbf{n}^{(0)} + \delta\mathbf{n}(x)$ with $\delta\mathbf{n}$

[3]see: Landau & Lifshits, Statistical Physics, Part I, § 140

transverse to $\mathbf{n}^{(0))}$. Plugging this into (13) and expanding to the lowest nonvanishing order in $\delta\mathbf{n}(x)$, one obtains energy of the form $E(\delta\mathbf{n}) = \frac{1}{2}\int \mathcal{K}(\nabla\delta\mathbf{n})^2$. (This expression is schematic, in fact $\mathcal{K}$ is a tensor with some dependence on $\mathbf{n}^{(0))}$, but this is good enough for the moment.) Expanding $\delta\mathbf{n}(x)$ in Fourier harmonics, $\delta\mathbf{n}(x) = \int \delta n_k e^{i\mathbf{k}\cdot\mathbf{x}} d^3/(2\pi)^3$, obtain

$$E(\delta\mathbf{n}) = \frac{1}{2}\int \mathcal{K}(\mathbf{k}\cdot\delta\mathbf{n}_k)^2 d^3/(2\pi)^3 \tag{14}$$

Using the equipartition theorem, one can estimate thermal fluctuations in each mode $\overline{|\delta\mathbf{n}_k|^2} \propto T/\mathcal{K}k^2$ and consider thermodynamics of the system pretty much like for vibrational modes above. (To be discussed later in more detail.)

Heisenberg ferromagnet: Magnetism arises due to exchange interaction of electron spins. Typically, the spins involved in magnetic ordering come from the electrons localized on crystal lattice sites, so that one can ignore orbital electron dynamics and focus on the spins and their interactions. The simplest model describing ferromagnetism, known as the Heisenberg model, involves Pauli spin operators: $\mathcal{H} = -\frac{1}{2}\sum_{r\neq r'} J(r-r')\,\hat{\mathbf{s}}_r\cdot\,\hat{\mathbf{s}}_{r'}$, where $\hat{\mathbf{s}}_r = \sigma_1, \sigma_2, \sigma_3$ and $J(r-r') > 0$ is spin exchange interaction.

Instead of this full quantum Hamiltonian we shall consider a classical Heisenberg model

$$\mathcal{H} = -\frac{1}{2}\sum_{r\neq r'} J(r-r')\,\mathbf{S}_r\cdot\,\mathbf{S}_{r'} \tag{15}$$

Here $\mathbf{S}_r$ is a unit vector describing average spin polarization in the system at the point r. This model describes a large spin limit of the quantum problem. The classical and quantum models have identical symmetry properties, the same set of low energy modes, and hence the same thermodynamical properties.

The Hamiltonian (15) is invariant under spin rotations. This is a bit more tricky than in previous examples, since this is not a physical space rotation, but rather a rotation in an "internal space." The ground state is described by uniform magnetization with arbitrary orientation. Thus there are infinitely many ground states, and we have the same sort of continuous degeneracy as before.

To find the enrgy of the soft modes, we consider a weakly inhomogeneous spin field $\mathbf{S}_r = \mathbf{S}^{(0)} + \delta\mathbf{S}_r$, plug it in the energy (15) and expand in $\delta\mathbf{S}$. This calculation is most easily carried out by rewriting Eq.(15) as

$$\mathcal{H} = \frac{1}{4}\sum_{r\neq r'} J(r-r')\,(\mathbf{S}_r - \mathbf{S}_{r'})^2 = \frac{1}{4}\sum_{r\neq r'} J(r-r')\,(\delta\mathbf{S}_r - \delta\mathbf{S}_{r'})^2 \tag{16}$$

(we used that $\mathbf{S}_r^2 = 1$ and added a constant term $\sum_r J(0)\mathbf{S}_r^2$). As long as $J(r-r')$ falls rapidly, the points r and r' are close, and for slowly varying field configuration one can expand $\mathbf{S}_r - \mathbf{S}_{r'} = (r_k - r'_k)\nabla_k\mathbf{S} + O((r-r')^2)$. This gives

$$E(\mathbf{S}) = \frac{1}{2}\sum_r J_{kk'}(\nabla_k S_j)(\nabla_{k'} S_j) = \frac{1}{2}\int_r J_0(\nabla\mathbf{S})^2 d^3r \tag{17}$$

with $J_{kk'} = \frac{1}{2}\sum_r J(r) r_k r_{k'}$, $J_0 = \frac{1}{6}\sum_r J(r) r^2$. Ther last expression in Eq.(17), rotationally invariant under independent spin and space rotations, applies to sufficiently symmetric situations, such as spins in a cubic lattice with exchange interaction being a function of distance only, when $J_{kk'} = J_0 \delta_{kk'}$.

This example illustartes how *a classical field description emerges* from a microscopic model. We start from functions of a dicrete variable, spins on a lattice, with interaction $J(r - r')$ that typically takes place on short length scale, $|r - r'|$ or the order of lattice spacing. By considering slowly varying perturbation field configurations which locally look like one of (continuously degenerate) ground states, we arrive at a macroscopic description involving functions $\mathbf{S}_r$ of a continuous variable $r \in R^3$ with an effective Hamiltonian (17). It is characteristic for the situations with continuous symmetry of the order parameter that the Hamiltonian is written in terms of gradients.

Alternatively, one can derive (17) using Fourier representation. We expand $\mathbf{S}_r = \int \mathbf{S}_k e^{i\mathbf{k}\cdot r} d^3k/(2\pi)^3$, and rewrite (15) as

$$E(\mathbf{S}) = \frac{1}{2} \int J(k)\, \mathbf{S}_k \cdot \mathbf{S}_{-k} \frac{d^3k}{(2\pi)^3} \tag{18}$$

where $J(k)$ is a Fourier transform of $J(r)$. Note that since the spins sit on lattice sites, the Fourier transform is defined as for functions of a discrete variable. Because of that, the integral over k in Eq.(18) runs not over the entire k space but only over a domain $-\pi/a < k_i < \pi/a$ with a the lattice period.

Expanding Eq.(18) in $\delta\mathbf{S}$, we obtain

$$E(\delta\mathbf{S}) = \frac{1}{2} \int (J(k) - J(0))\, \delta\mathbf{S}_k \cdot \delta\mathbf{S}_{-k} \frac{d^3k}{(2\pi)^3} \tag{19}$$

For long wavelength spin waves, we can expand $J(k) - J(0) = J_0 k^2 + O(k^4)$. Keeping only the term $J_0 k^2$ and going back to the real space, we have $\frac{1}{2} \int J_0 (\nabla \delta\mathbf{S})^2 d^3r$. However, since the background state is constant, $\nabla \mathbf{S}^{(0)} = 0$, this can be brought to the form

$$E(\mathbf{S}) = \frac{1}{2} \int J_0 (\nabla \mathbf{S})^2 d^3r \tag{20}$$

This expression gives the energy of a weakly inhomogeneous spin-polarized state.

Let us comment on the analogy with the liquid crystal energy (13). There seems to be a similarity, since the order parametr in both cases is a unit vector. The crucial difference is that in the liquid crystal case this vector defines orientation in the real physical space, while in the magnet problem it is a vector in the inner spin space. This results in a different form of the energy: a single term in (20) versus three independent terms in (13). Indeed, the only exprssion quadratic in the graduients $\nabla\mathbf{S}$ and invariant under *independent* real and spin rotations is $(\partial_i S_j)^2$, which is precisely the energy density (20).

The analysis of thermodynamics is quite analogous to the liquid crystal case (see also the homework problem 2, PS#1). We shall come back to the problem (20) again later.

Incommensurate crystals is an example of even more exotic symmetry.

Density modulation with incommensurate periods. In 1D case, say,

$$n(x) = A\cos(k_1 x) + B\cos(k_2 x + \theta) \tag{21}$$

Invariance of the system energy with respect to changes of the phase θ by an overall constant. The low energy states are described by slowly varying phase $\theta(x)$ in Eq.(21). The energy is given by a gradient expansion of the form

$$E(\theta) = \frac{1}{2}\int K(\partial_x\theta)^2 dx \qquad (22)$$

These soft modes are called "phasons," since they describe phase fluctuations.

Phyasically, they correspond to one density wave sliding freely relative to the other one.

Talk about mercury chains in the material $Hg_{3-\delta}AsF_6$, the "alchemist gold."

1.4 Now, let us summarize

- **Emerging classical fields:** The macroscopic description of systems with broken symmetry is provided by a classical field, one or several functions in Euclidean space. This description is usually quite simple, while the microscopic origin of the ordering can be rather complicated.

- **Universality:** Many systems seemingly very difrerent microscopically have the same or very similar description in the macroscopic limit. Different universality classes differ mainly by the symmetry of the ordering and (usually in a less important way) by interactions.

- **Goldstone modes:** In the case of spontaneously broken continuous symmetry, the low energy excitations are described by weakly inhomogeneous order paramer field. The fluctuations of these modes govern the thermodynamic properties.

- **The phenomenolgical and microscopic approaches:** The form of the energy describing slowly varying fields can be deduced on the basis of symmetry by listing all possible invariants in the gradient expansion and carefully analyzing symmetry requirements. The constants in such phenomenolgical hamiltonians should be calculated from a microscopic approach. The relation of this energy functional to the microscopic Hamiltonian can be simple, as in the case of lattice vibrations and Heisenberg ferromagnet model, or very complicated, as in the case of liquid crystals or incommensurate crystals.