Chapter 15

Phonons, Bloch Waves; Spontaneous Symmetry Breaking

15.1 Translations on a Lattice

We have seen that symmetry groups may have different implications on the physics. The first we have seen is an "internal symmetry", global, manifested by multiplets of states which form the space acted upon by a representation of the group. Quite different is a local symmetry, which, although it is a much larger group, being a product of groups at each space-time point, does not have a corresponding map of different physical states into each other. Rather, through gauge invariance, it makes some of the apparent fields A^a_μ unphysical, so that the $4n$ fields A^a_μ (n is the dimension of the group) only describe $2n$ degrees of freedom, transversely polarized "photons".

Another form of symmetry's effect is given by the translation group. Consider a spatial cubic lattice with sites $\vec{x} = (n_x, n_y, n_z)a$, with $n_i \in \mathbb{Z}$, a the lattice spacing, and with a field ϕ on each site. If we think of this as an approximation to a relativistic field theory with Lagrangian density

$$\mathcal{L} = \frac{1}{2}\left(\partial^\mu\phi\right)\left(\partial_\mu\phi\right) - \frac{1}{2}\mu^2\phi^2 - \frac{1}{4}\lambda\phi^4,$$

the latticized Hamiltonian density is

$$\mathcal{H} = \frac{1}{2}\dot{\phi}^2_{\vec{n}} + \frac{1}{2a^2}\sum_s \left(\phi_{\vec{n}+s} - \phi_{\vec{n}}\right)^2 + W(\phi_{\vec{n}}),$$

where $W(\phi) = \frac{1}{2}\mu^2\phi^2 + \frac{1}{4}\lambda\phi^4$, and the $\sum_s$ means summing over the three directions x, y, z with $\vec{n} + s$ meaning the vector $(n_j + \delta_{js})$, that is, one of the nearest neighbors in each direction.

The same form is a standard Hamiltonian in solid state physics, although W need not be given by ϕ^2 and ϕ^4 terms there. (This limitation comes from requiring renormalizability for a relativistic continuum theory.)

Let us first ask what translational invariance imposes on the states of this system. Under a translation $\vec{n} \to \vec{n} + \vec{t}$, where $\vec{t}$ has integer components, implemented by an operator $U_{\vec{t}}$,

$$U_{\vec{t}}^{-1}\phi_{\vec{n}}\, U_{\vec{t}} = \phi_{\vec{n}+\vec{t}},$$

the Hamiltonian is invariant because it is a sum over all sites equally. We expect the states to transform as a sum of irreducible representations of the group

$$U_{\vec{t}}|\psi_j\rangle = \Gamma^k_{ij}(U_{\vec{t}})\,|\psi_i\rangle\,.$$

The translation group is Abelian, so all of its irreducible representations are one dimensional, because all of the $\Gamma(U)$'s commute and can be simultaneously diagonalized. The group is generated by the three translations by one lattice spacing, which must have unitary representations $\Gamma\left(U_{\vec{t}}\right) = e^{iak_jt_j}$. The $\vec{k}$ is a momentum. For an infinite lattice it may take on any value. But $k_j \longrightarrow k_j + \frac{2\pi}{a}$ has no effect on any of the fields. So both k's are the same representation of lattice translations.

It is possible to reformulate the Hamiltonian in terms of operators which transform more simply under translations. Let

$$q_{\vec{k}} = \sum_{\vec{n}} e^{i\vec{k}\cdot(a\vec{n})}\phi_{\vec{n}}$$

where we restrict $\vec{k}$ to the interval $\left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$. Then

$$\begin{aligned}\int_{-\pi/a}^{\pi/a} d^3k\, \dot{q}_{\vec{k}}\,\dot{q}_{-\vec{k}} &= \int_{-\pi/a}^{\pi/a} d^3k \sum_{\vec{n},\vec{n}'} e^{ia\vec{k}\cdot(\vec{n}-\vec{n}')}\dot{\phi}_{\vec{n}}\,\dot{\phi}_{\vec{n}'}\\ &= \sum_{\vec{n}}\sum_{\vec{n}'}\dot{\phi}_{\vec{n}}\,\dot{\phi}_{\vec{n}'}\left(\frac{2\pi}{a}\right)^3\delta_{\vec{n},\vec{n}'} = \left(\frac{2\pi}{a}\right)^3\sum_{\vec{n}}\dot{\phi}^2_{\vec{n}}\end{aligned}$$

so the momentum term can be easily reexpressed. Without the time derivatives the same thing holds, so the $\frac{1}{2}\mu^2\phi^2$ is no problem either.

Inverting, $\phi_{\vec n} = (a/2\pi)^3 \int_{-\pi/a}^{\pi/a} d^3k\, e^{-ia\vec k\cdot\vec n} q_{\vec k}$, so we see that

$$\phi_{\vec n+\vec s} - \phi_{\vec n} = \frac{a^3}{(2\pi)^3}\int_{-\pi/a}^{\pi/a} d^3k\, e^{-ia\vec k\cdot\vec n}\left(e^{-ia\vec k\cdot\vec s}-1\right) q_{\vec k},$$

so

$$\begin{aligned}\frac{1}{2a^2}\sum_{\vec n,s}\left(\phi_{\vec n+\vec s}-\phi_{\vec n}\right)^2 \quad &= \quad \left(\frac{1}{2\pi}\right)^6 \frac{1}{2a^2}\int d^3k\, d^3k' \sum_{\vec n} e^{-ia(\vec k+\vec k')\cdot\vec n} \\ &\qquad \left(e^{-ia\vec k\cdot\vec s}-1\right)\left(e^{-ia\vec k'\cdot\vec s}-1\right) q_{\vec k} q_{\vec k'}.\end{aligned}$$

But

$$\sum_{\vec n} e^{-ia(\vec k+\vec k')\cdot\vec n} = \left(\frac{2\pi}{a}\right)^3 \delta^3(\vec k+\vec k'),$$

so $\vec k' = -\vec k$, $\left(e^{-ia\vec k\cdot\vec s}-1\right)\left(e^{-ia\vec k'\cdot\vec s}-1\right) = 4\sin^2\left(\frac{a\vec k\cdot\vec s}{2}\right)$, so the gradient term is

$$\left(\frac{a}{2\pi}\right)^3 \frac{2}{a^2}\int d^3k \sum_s \sin^2\left(\frac{a\vec k\cdot\vec s}{2}\right) q_{\vec k} q_{-\vec k}.$$

We note that hermiticity of ϕ_n implies $q_{-\vec k} = q^\dagger_{\vec k}$. So we see that the Hamiltonian, except for the terms in W higher order than 2nd order in ϕ, are diagonal quadratic operators in $q_{\vec k}$, of a harmonic oscillator type. The quartic term gives a coupling interaction between different $q_{\vec k}$'s.

The $q_{\vec k}$ operators transform very simply under the translations:

$$U^{-1}_{\vec t} q_{\vec k} U_{\vec t} = \sum_{\vec n} e^{ia\vec k\cdot\vec n}\phi_{\vec n+\vec t} = \sum_{\vec n'} e^{ia\vec k\cdot(\vec n'-\vec t)}\phi_{\vec n'} = e^{-ia\vec k\cdot\vec t} q_k,$$

so U only changes the phase of $q_{\vec k}$.

The $q_{\vec k}$ and $\dot q_{\vec k}$, for each $\vec k$ separately, can be combined into harmonic oscillator raising and lowering operators $a^\dagger_{\vec k}$ and $a_{\vec k}$, which correspond to the creation and annihilation of quanta of momentum $\vec k$. The quadratic terms in the Hamiltonian become $\sum_{\vec k}\omega_{\vec k} a^\dagger_{\vec k} a_{\vec k}$, which simply counts the number of phonons of momentum $\vec k$, multiplies by the energy $\omega_{\vec k}$ of each, and sums. Invariance of a term in the Hamiltonian $\propto \prod_i q_{\vec k_i}$ requires $e^{-ia(\sum \vec k_i)\cdot\vec t} = 1$, or

$$\sum_i \vec k_i = \frac{2\pi}{a} \times \text{integer}.$$

So we have interactions of phonons with the total incoming momentum not conserved, but conserved modulo $2\pi/a$. If we write a momentum operator $\vec{P} = \sum_{\vec{k}} \vec{k} a^\dagger_{\vec{k}} a_{\vec{k}}$ we can show that

$$U_{\vec{t}} = e^{ia\vec{t}\cdot\vec{P}}.$$

$\vec{P}$ is not a conserved quantity, because only $U_{\vec{t}}$ are symmetries, not other translations by non-integer numbers of lattice spaces. But $\vec{P}$ is conserved modulo $2\pi/a$, so $U_{\vec{t}}$ is conserved.

The nuclei of a crystal lattice carry degrees of freedom which are displacements from the lattice points, but they are not fields defined for all $\vec{x}$, so the translational modes only involve integer numbers of lattice spaces. The electrons, however, at least the ones not tightly bound, need to be treated as fields and therefore dependent on $\vec{x}$ as a continuous variable. We can ask how the lattice translational invariance affects the wave functions $\psi(\vec{x})$ for an electron which experiences a periodic potential $V(\vec{x}) = V(\vec{x} + a\vec{t})$. Again the possible states can be decomposed into irreducible representations, which as the group is Abelian are one-dimensional and unitary, so $\psi(\vec{x} + a\vec{t}) = e^{ia\vec{k}\cdot\vec{t}}\psi(\vec{x})$. Then, if we write $\psi(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} u_{\vec{k}}(\vec{x})$, we see that $u_{\vec{k}}(\vec{x} + a\vec{t}) = u_{\vec{k}}(\vec{x})$, so the **Bloch function** $u_{\vec{k}}(\vec{x})$ is periodic on the lattice. But we must keep in mind that the electron wave function is not periodic.

As before, the irreducible representation $\vec{k}$ is defined only for $\vec{k}$ modulo the reciprocal (or *Bravais*) lattice, so is essentially defined only within the *Brillouin zone* ($k_j \in [-\frac{\pi}{a}, \frac{\pi}{a})$). But there may be several Bloch functions, in bands, for the same $\vec{k}$. For example, a free electron ($V = 0$) is trivially in a periodic potential, and has eigenfunctions $e^{i\vec{k}\cdot\vec{x}}$ for all $\vec{k}$, so when considered as Bloch functions with $\vec{k}'_j \in [-\frac{\pi}{a}, \frac{\pi}{a})$, the higher k values will be shown as higher energy states with the same $\vec{k}'$.

15.2 Spontaneous Symmetry Breaking

We will return to momenta and the translation group in a relativistic continuum theory later, only for the continuum. But first let us consider another symmetry.

The Hamiltonian

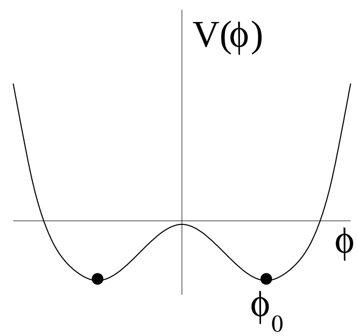
$$\mathcal{H} = \frac{1}{2}\dot{\phi}^2_{\vec{n}} + \frac{1}{2a^2}\left(\phi_{\vec{n}+\vec{t}} - \phi_{\vec{n}}\right)^2 + \frac{1}{2}\mu^2\phi^2_{\vec{n}} + \frac{1}{4}\lambda\left(\phi^2_{\vec{n}}\right)^2$$

is invariant under a global transformation $\phi_{\vec n} \to -\phi_{\vec n}$. In fact, if one considers $\phi_{\vec n}$ to be a vector in some N dimensional real vector space, with $\phi^2_{\vec n} := \sum_j (\phi_{\vec n})^2_j$, $\mathcal{H}$ is invariant under SO(N) global transformations on the ϕ's.

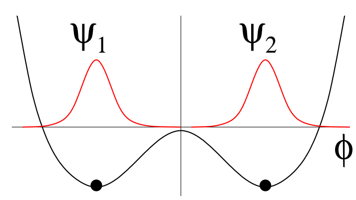
Consider the *classical* ground state of the system. Any time derivative or gradient only increases the energy, so the ground state is $\phi_{\vec n}$ = constant $=: \phi_0$, with

$$V(\phi) = \frac{1}{2}\mu^2\phi^2 + \frac{1}{4}\lambda\phi^4$$

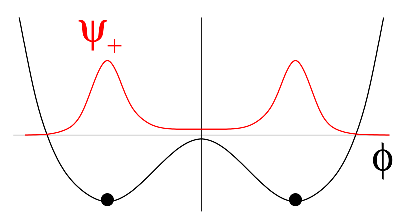
taking its minimum value at ϕ_0.



If μ^2 and λ are positive, the minimum is clearly at $\phi_0 = 0$, and this classical ground state is invariant under sign reversal or rotation of ϕ. If $\mu^2 < 0$, however, the potential has a local *maximum* at $\phi = 0$, with two degenerate minima at $\phi = \pm\phi_0 \neq 0$. If ϕ is a vector, this diagram is rotated into the bottom of a wine bottle, and the minimum becomes ring or sphere.

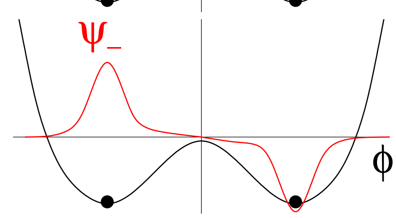


If we were talking about a one-dimensional quantum mechanics problem $H = \frac{p^2}{2m} - \frac{|\mu^2|}{2}x^2 + \frac{\lambda}{4}x^4$, the two classical ground states at $x = \pm\phi_0 = \pm\sqrt{|\mu^2|/\lambda}$ would become two approximate eigenstates ψ_1 and ψ_2 concentrated around the two minima. If there were no overlap, ψ_1 and $\pm\psi_2$ would be eigenstates of the same energy.



But as there is some overlap, the true eigenstates would be linear combinations

$\psi_1(x) + \psi_2(x)$	ground state
$\psi_1(x) - \psi_2(x)$	first excited state



with an energy separation proportional to the overlap between ψ_1 and ψ_2. ψ^+ has slightly lower energy than ψ^-, which bends a bit more.

For our lattice, there are also a set of degenerate classical ground states, with all $\phi_{\vec n} = \pm\phi_0$, but all the $\phi_{\vec n}$'s must be the same. The quantum mechanical states then have wave functions $\psi(\phi_1, \phi_2, \ldots)$ centered around $\phi_1 = \phi_2 = \cdots = \phi_V = \pm\phi_0$ if there are V points in our lattice. The overlap of these states, however, is approximately the V'th power of the single site overlap, V is likely to be very large, and for the infinite lattice limit, there is no overlap at all! And so the quantum system has a true degeneracy of eigenstates, including the ground state.

Consider a ferromagnet below the Curie point. The magnetic dipoles want to line up, but which way is immaterial. They must all line up in the same way, however, to get the lowest energy state.

Once the whole material is lined up, the possibility of a transition to one of the other degenerate vacuum states is an exponentially decreasing function of the volume of the system. So the statement that the states of the system form multiplets of the group becomes irrelevant — the relevant physical states are the ones close enough to the particular original ground state for transitions to be possible. The Hamiltonian still has a symmetry group, but the relevant states no longer transform as an irreducible representation of it. This is called **spontaneous symmetry breaking**.

A particularly interesting feature emerges when the symmetry group is a continuous one. Consider ϕ as an N-vector, and let ϕ_0 be the "vacuum" value. Then the Hamiltonian is invariant under a global symmetry $e^{i\omega^b L_b}$ with L_b the generators of the Lie algebra of SO(N). If we consider a local transformation $e^{i\omega^b(\vec{x})L_b}$, the Hamiltonian is invariant except for the gradient term, which gets a piece $\sim \vec{\nabla}\phi \cdot \vec{\nabla}\omega^b L_b \phi$. Then the energy of the state $e^{i\omega^b(\vec{x})L_b}|\Omega\rangle$ is

$$\langle\Omega| e^{-i\omega^b(\vec{x})L_b} H e^{i\omega^b(\vec{x})L_b} |\Omega\rangle = \langle\Omega| H + i[H, \omega^b L_b] - \frac{1}{2}[[H, \omega^b L_b], \omega^c L_c] + \cdots |\Omega\rangle .$$

The first term is just the ground state energy E_0. The second term is $\int d^3x \vec{\nabla}\omega^b(\vec{x}) \langle\Omega| \vec{\nabla}\phi(\vec{x})\Gamma(L_b)\phi(\vec{x}) + \text{h.c.} |\Omega\rangle$. As $\Gamma(L_b)$ is hermitean, the operator is $\vec{\nabla}(\phi\Gamma(L_b)\phi)$, which therefore vanishes as $\langle\Omega| \phi(\vec{x})\Gamma(L_b)\phi(\vec{x}) |\Omega\rangle$ is $\vec{x}$ independent by translational invariance. Therefore the leading term in ΔE is proportional to the integral over space of the square of the gradient of ω. If the variation of ω takes place over a region of length L, for a total fixed variation of $\Delta\omega$, $\nabla\omega \propto \Delta\omega/L$, and the region over which this energy density is increased is $\propto L$, so

$$\Delta E \propto L \times \left(\frac{\Delta\omega}{L}\right)^2 \propto \frac{1}{L} \propto k$$

if $\omega(x)$ varies roughly as e^{ikx}. Thus if the variation is slow enough, the energy of this state differs from the ground state by arbitrarily little, proportional to the momentum of the "spin-wave", which is rotating the ϕ field with a gentle long wavelength. The added energy can be attributed to this spin-wave or **Goldstone boson**, which has an energy proportional to its momentum as would be expected for a zero-mass particle.

Let's consider this more generally. Suppose the theory is invariant under a Lie group G with Lie algebra $\mathfrak{G}$, but the vacuum state $|\Omega\rangle$ is invariant only under a subgroup K with Lie Algebra $\mathfrak{K}$. If the fields transform under a *constant* transformation $\phi_a \to \left(e^{i\omega^j\Gamma(L_j)}\right)_{ab}\phi_b \approx \phi_a + \alpha\Delta_a(\phi)$ acting on $|\Omega\rangle$ the energy of the transformed vacuum state[1] becomes

$$V(\phi_a + \alpha\Delta_a(\phi)) \approx V(\phi_a) + \alpha\Delta_a(\phi)\frac{\partial V(\phi)}{\partial\phi_a} = V(\phi_a)$$

because the theory, and V, must be invariant under G. So

$$\Delta_a(\phi)\frac{\partial V(\phi)}{\partial\phi_a} = 0$$

for all fields ϕ. Differentiate with respect to ϕ_b and set ϕ to its value in the vacuum state ϕ_0:

$$\left.\frac{\partial\Delta_a}{\partial\phi_b}\right|_{\phi_0}\left.\frac{\partial V}{\partial\phi_a}\right|_{\phi_0} + \Delta_a(\phi_0)\left.\frac{\partial^2 V}{\partial\phi_a\,\partial\phi_b}\right|_{\phi_0} = 0.$$

But the first term vanishes as $\left.\dfrac{\partial V}{\partial\phi_a}\right|_{\phi_0} = 0$ because ϕ_0 minimizes V. So

$$\Delta_a(\phi_0)\left.\frac{\partial^2 V}{\partial\phi_a\,\partial\phi_b}\right|_{\phi_0} = 0. \qquad (15.1)$$

Note that $m^2_{ab} = \dfrac{\partial^2 V}{\partial\phi_a\,\partial\phi_b}$ is a mass term in the lagrangian. Now if our $\omega^j L_j$ lies within $\mathfrak{K}$ and leaves the vacuum state ϕ_0 invariant, $\Delta_a(\phi_0) = 0$ and we learn nothing from (15.1). But if $\omega^j L_j \notin \mathfrak{K}$, $\Delta_a(\phi_0)$ is a nonzero vector in the space of ϕ, and then (15.1) tells us that the mass matrix acting on $\Delta_a(\phi_0)$

[1] V can represent the energy of a full quantum state $|\phi\rangle$ for a $\phi(x)$ field configuration.

vanishes, so that this corresponds to a massless excitation. Thus there is one massless Goldstone boson for each dimension in the coset space $\mathfrak{G}/\mathfrak{K}$.

We have not exhausted the ways symmetries can work their magic, however. We see that a broken symmetry can give rise to massless scalar particle for directions in the Lie algebra. We previously saw that gauge theories gave massless vector particles for each direction in a Lie algebra. The Higgs mechanism combines these two — and the massless vectors eat the Goldstone bosons, gaining the third degree of freedom which allows them to become fat, *i.e.* massive. This is the basis of the electroweak interactions, with the weak vector particles $W^\pm$ and Z^0 getting mass from the Higgs field, while the photon retains its masslessness in the direction of the unbroken Maxwell gauge invariance. Before we do this, however, let us consider what happens in more detail in SO(N) scalar field theory.