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1991 J. Phys. A: Math. Gen. 24 5273

(http://iopscience.iop.org/0305-4470/24/22/011)

J Phys A Math Gen 24 (1991) 5273–5281 Printed in the UK

Spontaneously broken symmetries

Rudolf Peierls

Nuclear Physics Laboratory, University of Oxford, Keble Road, Oxford OX1 3RH, UK

Received 4 July 1991

Abstract. This is an attempt to clarify the structure of spontaneous symmetry breaking It is shown that there are two types of situation In one, called here SBS1, a symmetric ground state is degenerate with an asymmetric one, in the other, SBS2, the ground state belongs to a representation other than the identical one Some cases which look like spontaneous symmetry breaking are in fact symmetry-breaking approximations

1. Introduction. The classical case

This paper does not claim to contain any new results, but is intended only to clarify the basic logic. 'Spontaneously broken symmetry' denotes a situation in which the Hamiltonian of a system possesses certain symmetries, but in which the usual description of the system in the absence of excitations (the 'vacuum') does not have the same symmetries, i.e does not belong to the identical representation of the relevant symmetry group. The simplest example of a spontaneously broken symmetry (SBS) is 1D motion in a potential with two equal minima, say at $x=a$ and $x=-a$. The symmetry is the operation $x\to -x$ The problem arises in one degree of freedom of molecules such as sugar Classically it is obvious that there are two equilibrium positions, and the system will settle in one or the other, thus breaking the symmetry.

2. The two-well problem in quantum mechanics

In quantum mechanics we know from general theorems that the ground state, unless it is degenerate, must belong to an irreducible representation of the symmetry group, i.e. it must be either even or odd in x, and we know that the ground state of a one-body problem has a nodeless wavefunction, so it is even The ground state represents a situation in which the particle is with equal probability in either well The first excited state will in general be odd. Its energy lies above the ground state by an amount which depends on the amplitude for penetrating the barrier between the two minima. So the energy difference is small if the barrier is high or the mass is large.

Consider for a moment the limit in which energy difference between the two states is zero. We then have freedom to choose any linear combination of the two degenerate wavefunctions, in particular we may choose one which vanishes in one of the wells, and therefore breaks the symmetry, as in the classical case. However, as long as the system is isolated, there is nothing to compel us to make that choice, and on the face of it it seems rather unnatural to do so.

If an external perturbation acts on the system, however weak, the eigenfunctions must be found close to the 'eigenfunctions of zero-order approximation', i.e. those

0305-4470/91/225273+09$03 50

among the degenerate eigenfunctions which in the degenerate space diagonalize the perturbation. Now any realistic perturbation which splits the degeneracy will act differently on a particle in the left-hand well from one on the right, and therefore the correct zero-order eigenfunctions are those which localize the particle in either well and thus break the symmetry

Now turn to the realistic case, in which there is no degeneracy, and on the face of it we would have to use the symmetric eigenfunction to describe the ground state, and this indeed has to be the starting-point for studying a perturbation which is weaker than the splitting between the even and the odd state. But for large mass or high barrier this splitting is exponentially small, and such weak perturbing forces are not very interesting. If the effect of the force is comparable with the splitting one has to use the method of almost degenerate eigenfunctions, and if the perturbing potential is larger than the splitting this amounts to treating the two states as degenerate Again any realistic perturbation requires the localized, i.e. symmetry-breaking, wavefunction, although this is not strictly an eigenfunction of the unperturbed Hamiltonian, i.e it is not strictly stationary.

We might ask what would be an example of a perturbation for which the zero-order eigenfunctions would be the ones respecting the symmetry. A little algebra shows that this requires

$$V_{11} - V_{22} - V_{21} + V_{12} = 0 \tag{1}$$

and

$$V_{21} + V_{12} \neq 0 \tag{2}$$

where the subscripts 1 and 2 denote the wavefunctions in the right- and left-hand well (the sum and difference of the even and odd solutions). For a real local potential $V_{12} = V_{21}$, and then from (1) $V_{11} = V_{22}$.

Then (2) shows that the perturbing potential must act in the region in which ψ_1 and ψ_2 overlap, i.e. inside the barrier, where they are both small. Such potentials are not likely to arise in practice.

The symmetry-breaking state may also arise if we observe the position of the particle, during a time short compared to $\hbar$ divided by the level splitting. This observation will show it on the left, or the right-hand side, i.e. in an asymmetric state. This is not a stationary state, but the error in the energy is not seen during the short time. If we wait long enough we shall see the particle oscillating between the two wells.

This is the situation of the optically active molecules, such as sugar. A single molecule of right-handed sugar in isolation will have a small, but finite probability of making a transition to the left-handed form and vice versa. But this probability is so small that over reasonable times we may disregard it. So we are led to a situation in which we think of sugar as normally right-handed or left-handed, and not the even or odd combination, although the latter are the correct stationary states. Also an observation of the structure directly by a high-resolution microscope, or indirectly through the optical activity, we will show the molecule in the right- or left-handed form, thus breaking the symmetry.

3. Other simple cases

An equally trivial example is the centre-of-mass motion of any system such as a crystal. The Hamiltonian has translational symmetry, and the exact ground state is one in

which the wavefunction is spread over all space, with zero momentum. Above it in energy starts a continuous spectrum of different momenta. If the crystal is macroscopic a very small energy interval contains a big enough spread of momentum to allow the formation of a wavefunction which localizes the centre of mass of the crystal to well within an atomic spacing. So again the crystal we handle is represented by a localized function, which breaks the symmetry. The situation is evidently quite similar with rotational symmetry

We can again ask what perturbation would lead to the momentum eigenstates as zero-order functions. It would have to be something like an infinitely extended uniform magnetic field, with the crystal carrying an overall charge In practice crystals and other solid objects which we study are usually fixed to a bench or held in our hand, spoiling the translational symmetry. But when we observe a freely falling snowflake it has a definite position and is not spread over all space

The common features of these systems are (i) the near-degeneracy of states of different symmetry, and (ii) the tendency of realistic perturbing effects, or of methods of observation, to select localized, and thus symmetry-breaking states. I shall refer to this situation as a spontaneously broken symmetry of the first kind (SBS1). It is evidently misleading to say that in cases of broken symmetry 'the ground state is not an eigenstate of the original [symmetry] group' (Anderson 1990).

4. Symmetry-breaking approximations

When we are concerned with the rotation of an isolated molecule, it is not large enough for the above considerations to apply, and indeed separate levels with definite rotational quantum numbers, i.e. distinct representations of the rotation group, are seen in band spectra. Whether we should treat a molecule as having a (nearly) specified orientation, or a specified angular momentum, depends on the context. In particular, collisions may be so fast that the time during which the colliding molecules interact is short, and the resulting energy uncertainty greater than the spacing of the rotational levels. We may then regard a number of rotational levels as degenerate, and attribute to the molecule roughly specified orientation

A more extreme situation arises in nuclear physics. A nucleus is not large or heavy enough for different states of translation or rotation to be near-degenerate. No perturbation that is commonly encountered would be strong enough to mix different states of translation or rotation sufficiently to treat the nucleus as having a fixed position or orientation. (However, this may be the case in short collisions, as in the molecular case mentioned above.) The observed spectra again show clearly defined rotational levels

However, another consideration arises here: it is often convenient to use wavefunctions which break the symmetry as approximations to the correct ones. This is because this allows us to incorporate by very simple means correlations which are more important for the energy than the symmetry. For example, the Hartree–Fock method (or its refinement by the Brueckner–Bethe method) starts from a potential well in a fixed position, thus violating the translational symmetry; a deformed well also violates rotational symmetry. The advantage of the model is that it allows us to use the Hartree–Fock solution as a first approximation. If we wanted to preserve the translational symmetry in the Hartree–Fock method, we would have to make a determinant of plane waves, which would be useless as an approximation. The point is that using

the Hartree–Fock method with plane waves excludes correlations between the positions of the nucleons, which should be located closely together in space.

This is not a situation in which the symmetry is spontaneously broken. We consciously use a wavefunction which is deficient by violating the symmetry. This fault shows up in the shell model by the appearance of spurious states, which represent the oscillation of the centre of mass of the nucleus relative to the centre of the fictitious well. This situation clearly cannot be described as spontaneously broken symmetry. I shall in the following refer to it as a 'symmetry-breaking approximation' (SBA).

A similar situation exists when we use a deformed well as a starting-point for describing a nucleus. This violates the rotational symmetry, which is experimentally evident in the spectrum showing states with angular momentum quantum numbers. Here again using a spherical well would, in the Hartree–Fock method, ignore the correlations in angle. In a deformed well, if one nucleon is far out in one direction, others are likely to be in that same (or opposite) direction. We again have an SBA, in which we trade a symmetry for the advantage of including, in Hartree–Fock, the angular correlations.

A purist might argue that the distinction between SBS1 and SBA is purely quantitative, a question of the energy difference between states of different symmetry relative to the kind of perturbing forces to be encountered. However, the situations of, say, the sugar and the deformed nucleus are so different that it is sensible to use different names for them. There may, of course, be borderline cases between these categories.

5. Another form of symmetry breaking. Ferromagnetism

All the examples of symmetry breaking described so far have the common feature that the state we use for the description of the system does not belong to an irreducible representation of the symmetry group. There is a different class of situation, which shows the typical signs of broken symmetry, and should be included under that heading. That is the case in which the ground state (or 'vacuum') belongs to a representation of the symmetry group other than the identical one. In that case all excitations (or particles) behave as if they did not have the full symmetry. I shall refer to this as spontaneously broken symmetry of the second kind (SBS2).

An example is a ferromagnet, which was the original *Schulbeispiel* of a spontaneously broken symmetry. This is a lattice of N atoms, each with spin s, with forces trying to align the spins, so that the ground state has $J = Ns$, and the total component in, say, the z direction is Ns. (This description ignores magnetic interactions and other effects; it is rather a mathematical ferromagnet, but this will serve our purpose.) Thus the ground state is not symmetric under the spin rotational group, but it belongs to an irreducible representation of the group.

Accordingly the excitation spectrum has lost symmetry. For instance, the state generated by applying the operator $J_z = \Sigma\, s_{nz}$ to the ground state (which is of course the state with $M = J - 1$) has zero excitation energy. In the limit of infinite N, i.e. for a ferromagnet filling all space, this state becomes the Goldstone boson. Indeed it is easy to see that the proof of the Goldstone theorem depends only on the existence of a group element which does not leave the ground state invariant.

Anderson (1990) prefers not to regard ferromagnetism (and presumably other cases of SBS2) as cases of broken symmetry, because the spectrum of Goldstone bosons does not have a singularity at infinite wavelength, as in the case of phonons. This is largely

a semantic question, but it seems convenient to include these cases among the broken symmetries.

6. Antiferromagnetism

The situation of an antiferromagnet is more complicated. (Anderson 1990 has pointed out this qualitative difference.) Assume a crystal of $2N$ atoms, each with spin s, can be divided into two equivalent sublattices. The forces tend to make the spins of neighbouring atoms opposite, so that the spins in each sublattice tend to be parallel, and the two sublattices have opposite magnetization. No exact solution is available.

This system again has rotational symmetry, and the ground state belongs to the identical representation, i.e. the total spin is $S=0$. In addition, the system allows a translation which interchanges the two sublattices (if the crystal is large enough to ignore surface effects). The ground state will be even or odd under this transformation. We are interested in a state in which one sublattice, say a, has positive spin component is the reference direction, and the other, b, has a negative component. This state breaks both symmetries. It is not easy to produce it by an external field, because it would have to be a field which acts in opposite directions on the atoms in the two sublattices. However, such a state can be reached by observation, for example by elastic neutron scattering, observing the phase of the scattered wave.

This is not a stationary state, and in due course will change to its partner under the symmetries. I have not been able to find a reliable estimate of the rate of change, but I conjecture it to be quite long in the macroscopic case, since the transition requires every spin in the crystal to flip. Since the Hamiltonian contains only terms which change the spin components of two neighbouring atoms by one unit, this involves many virtual intermediate steps. This somewhat hand-waving argument suggests that the switch takes a very long time, and that the cost in energy of the asymmetric state is low.

In other words, this is again a case of SBSI, though I cannot give an estimate of the relevant small energy difference.

7. Superconductivity

Next consider the case of a superconductor, for which it is often claimed that the gauge invariance is spontaneously broken. Global gauge invariance guarantees, in particular, conservation of the number of electrons, while the BCS approximation to the ground state is a superposition of states with different electron numbers. Such superpositions cannot form the exact state of the system because the electron number is strictly conserved. Indeed this is a typical case of SBA. What correlation does this approximation help us to enforce? The characteristic features of the BCS ground state wavefunction are: (i) the electrons are coupled in pairs, each pair being formed, with zero momentum, from states near the edge of the Fermi distribution; (ii) the state function is symmetric between the pairs. It is the second condition which is difficult to implement while keeping a fixed particle number, so that it pays to trade the symmetry for the convenience of ensuring this correlation, a typical case of SBA.

One can illustrate these statements by applying the idea to the BCS ground state wavefunction (see Schrieffer 1964, equation (2.23)):

$$\psi_0 = \text{constant} \prod_k (1 + g_k b_k^+)|0\rangle \tag{3}$$

where

$$b_k^+ = c_{k\uparrow}^+ c_{-k\downarrow}^+ \tag{4}$$

is the operator creating a pair, and $|0\rangle$ is the vacuum. The function (3) evidently contains all possible numbers of pairs and therefore violates global gauge invariance.

We can project this state on the space of a fixed electron number, say $2N$, by selecting from the expression (3) terms of order g^N. This projected function evidently conserves global gauge invariance. I shall not discuss the question of local gauge invariance.

The projected function also preserves the structure of the pairs. For current-carrying states, in which the BCS pairs are defined with non-zero momentum, which may also depend on position, the same features are preserved.

This projected function is much harder to work with, and a direct evaluation of the energy would be difficult, but it is easy to see that it has approximately the same expectation value of the energy as the BCS function. To see this, write

$$\psi_0 = \sum_N \psi_{0N} \tag{5}$$

where ψ_0 is the BCS function (3), and ψ_{0N} its part containing just N pairs. Since the Hamiltonian conserves the number of electrons, we can write for the BCS energy

$$W = \frac{\langle\psi_0|H|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle} = \frac{\Sigma\langle\psi_{0N}|H|\psi_{0N}\rangle}{\Sigma\langle\psi_{0N}|\psi_{0N}\rangle} \tag{6}$$

which is the weighted average of the W_{0N}. The weights will be concentrated in a region around the mean value of N, say N_0 with a spread of about $\sqrt{N_0}$. For large N_0 the average W varies slowly with N_0 over that region, and therefore the W_{0N} must also vary slowly and be nearly equal to their weighted average.

A related question is how are we to understand the solution for quasiparticles as an approximation to a wavefunction conserving global gauge invariance. In the BCS definition of a quasiparticle state

$$\psi_p = (u_p c_p - v_p c_{-p}^+)\psi_0. \tag{7}$$

Insert (5) in (7) and collect terms of the same electron number:

$$\psi_p = \sum_N \{u_p c_p \psi_{0,N+1} - v_p c_{-p}^+ \psi_{0,N}\} \equiv \Sigma \psi_{p,N}. \tag{8}$$

The expectation value of the energy for the BCS state can therefore be expressed as

$$\frac{\langle\psi_p|H|\psi_p\rangle}{\langle\psi_p|\psi_p\rangle} = \frac{\Sigma\langle\psi_{p,N}|H|\psi_{p,N}\rangle}{\Sigma\langle\psi_{p,N}|\psi_{p,N}\rangle} = \frac{\Sigma_N \rho_{p,N} E_{p,N}}{\Sigma_N \rho_{p,N}}. \tag{9}$$

It is plausible that, for large N, the $E_{p,N}$ and $\rho_{p,N}$ vary slowly with N, so that the $E_{p,N}$ may be taken to equal their average, E_p, the BCS value.

The direct evaluation of the norms of the $\psi_{p,N}$ is fairly easy, but that of the diagonal elements of the Hamiltonian is complicated. It would have been quite impossible to find the solution by working within a symmetry-conserving framework. Applications and refinements of the theory would also become much less transparent.

These arguments seem to indicate that it is a good approximation to work with (3) or its generalization, although it does not describe a physically possible state. It clearly follows that this is not a case of spontaneously broken symmetry, but a symmetry-breaking approximation.

8. The Higgs mechanism

The most important case of SBS in particle physics is the Higgs mechanism. I have not been able to arrive at a complete understanding of the role of SBS in this, and the discussion in this section does not clarify the picture completely.

To start with, we consider the equation of the Higgs field by itself, not interacting with any other fields. We can then, of course, deal only with global gauge invariance The Lagrangian of the Higgs field may be written

$$\mathfrak{L} = \int d^3r \{\tfrac{1}{2}(\dot{\phi}^* \dot{\phi} - \nabla\phi^* \cdot \nabla\phi) - U(\phi^* \phi)\} \tag{10}$$

where U is a function which has a minimum, U_0, for some value, say v^2, of its argument. For clarity we shall assume that the integral is taken over a finite volume V with cyclic boundary conditions. If we write

$$\phi = R\, e^{i\theta} \tag{11}$$

where, of course, R and θ are real functions of the space coordinates, global gauge invariance means that $\mathfrak{L}$ is invariant against a constant shift in θ. It is tempting to change to R and θ as variables, but this leads to nonlinear equations, whose quantization is very difficult.

It is therefore usual to assume that ϕ is approximately real, and introduce real variables σ and τ by

$$\phi = v + \sigma + i\tau \tag{12}$$

neglecting terms higher than the second in σ and τ, since we want to test the hypothesis that ϕ can remain approximately real. We then expand:

$$\sigma = \sum a_k\, e^{ik\cdot r} \qquad \tau = \sum b_k\, e^{ik\cdot r}. \tag{13}$$

Inserting in $\mathfrak{L}$, finding the canonical conjugates to the a and b, forming the Hamiltonian and applying the quantum rules, we find

$$\langle\psi|\hat{H}|\psi\rangle = \tfrac{1}{2}\sum \left[(c^2\hbar/V)\left\langle \left|\frac{\partial\psi}{\partial a_r}\right|^2 + \left|\frac{\partial\psi}{\partial b_k}\right|^2 \right\rangle + V\langle |ka_k|^2 + |kb_k|^2\rangle \right]$$
$$+ VU_0 + 2VU''v^2 \sum |a_k|^2. \tag{14}$$

We are interested in τ, since from (11) and (12), to a sufficient approximation,

$$v\theta = \tau. \tag{15}$$

The average value of τ is given by b_0, and the only term in the Hamiltonian (14) containing b_0 is $\langle|\partial\psi/\partial b_0|\rangle^2$. Clearly, therefore, the state of minimum energy must have a state function which is independent of b_0. For such a state our approximation is not valid, because b_0, and therefore θ, is not restricted to small values. There is little doubt, however, that the correct ground state will have a state function independent of θ, thus being invariant under a global gauge transformation.

We may compare its energy with that of a state in which θ stays close to zero, e.g. if the b_0 dependence of ψ is a Gaussian:

$$\exp -\tfrac{1}{2}\alpha b_0^2 \tag{16}$$

the energy is increased only by

$$\delta E = c^2\hbar^2\alpha/V \tag{17}$$

which vanishes in the limit of infinite volume. The situation is therefore similar to that of the translation of a large solid; except that the limit $V\to\infty$ is physically exact, and not an approximation. We therefore have the degeneracy required for SBSI. It follows that we *may* choose the asymmetric or the symmetric state, but there is at this stage no evident reason why we *must* choose the asymmetric one.

Next we shall consider the Higgs field in the presence of an Abelian gauge field. I shall follow the presentation by Cheng and Li (1984). The basic Lagrangian density is

$$L = \tfrac{1}{2}[(D_\mu\phi)^+(D^\mu\phi)] - U(\phi^+\phi) - \tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} \tag{18}$$

with

$$D_\mu = \frac{\partial}{\partial x^\mu} - \mathrm{i}gA_\mu \qquad F_{\mu\nu} = \frac{\partial A_\nu}{\partial x^\mu} - \frac{\partial A_\mu}{\partial x^\nu}. \tag{19}$$

Writing

$$\phi = \frac{1}{\sqrt{2}}(v+\eta)\,\mathrm{e}^{\mathrm{i}\theta} \tag{20}$$

one can introduce the 'unitary gauge' by writing

$$\phi^u = \phi\exp(-\mathrm{i}\theta) \qquad B_\mu = A_\mu - \frac{1}{g}\frac{\partial\theta}{\partial x^\mu}. \tag{21}$$

This leads to the 'unitary Lagrangian density'

$$L^u = \frac{1}{2}\left|\frac{\partial\eta}{\partial x^\mu} - \mathrm{i}gB_\mu(v+\eta)\right|^2 - U(v+\eta) - \frac{1}{4}\left(\frac{\partial B_\nu}{\partial x^\nu} - \frac{\partial B_\mu}{\partial x^\mu}\right)^2 \tag{22}$$

In this form apparently no gauge-dependent assumption has been made, and it looks as if no symmetry has been broken. The Lagrangian (22) is to be interpreted with the assumption that in the vacuum η and B are zero. It is sometimes believed that the fact that the B field has a non-vanishing mass shows by itself that the gauge invariance has been broken. This, however, does not follow. A gauge invariant field by itself cannot have a mass, but if it is coupled to other fields it may well do so. For an example, see Anderson (1963).

It should be noted, however, that after quantization the Lagrangians (18) and (22) are not equivalent. If we apply the canonical formalism to (18) the time derivative of θ does not commute with θ, and therefore the differentiation of the exponential implied in the transformation becomes more complicated, and in fact singular. Therefore, starting from the quantized form of (18) it is not possible to derive (22). We may, of course, regard (21) as a classical transformation, leading to (22), and then apply the canonical formalism. This is a different theory.

In reality one is not concerned with the Abelian case, but with a Higgs field which is an isodoublet, and with a Lagrangian which is invariant under $SU(2) \times U(1)$. The $U(1)$ part of the symmetry is like the Abelian case discussed above. The $SU(2)$ symmetry is isomorphic with the rotational symmetry of an $s = \frac{1}{2}$ spinor. Thus the vacuum expectation of the Higgs field, and therefore the vacuum itself, belong to a representation of the symmetry other than the identical one. In this respect the Higgs mechanism involves a symmetry breaking of the second kind, in full analogy with ferromagnetism.

The whole mechanism therefore seems to involve both SBS1 and SBS2, but I have failed to clarify the SBS1 part.

Acknowledgments

The author would like to acknowledge helpful suggestions and constructive criticism from I J R Aitchison, P W Anderson, B Buck, P K Kabir, S Mandelstam, K W H Stevens and R B Stinchcombe.

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