

Spontaneous symmetry breaking in quantum mechanics

Jasper van Wezel and Jeroen van den Brink

Institute-Lorentz for Theoretical Physics, Universiteit Leiden, P. O. Box 9506, 2300 RA Leiden, The Netherlands

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We present a mathematically simple procedure to explain spontaneous symmetry breaking in quantum systems. The procedure is applicable to a wide range of models and can be easily used to explain the existence of a symmetry broken state in crystals, antiferromagnets, and even superconductors. It has the advantage that it automatically brings to the fore the main players in spontaneous symmetry breaking: the symmetry-breaking field, the thermodynamic limit, and the global excitations of a “thin” spectrum. © 2007 American Association of Physics Teachers. [DOI: 10.1119/1.2730839]

I. INTRODUCTION

In quantum mechanics symmetry has a much more powerful role than in classical mechanics. Translational invariance in a classical system causes momentum to be conserved; in quantum mechanics it immediately implies that all eigenstates of the Hamiltonian are spread out with equal amplitude over all of space. It could be argued that because a chair is built of many microscopic particles that all obey the rules of quantum mechanics, the chair as a whole should also respect the symmetry of its Hamiltonian and be spread out over all of space. Clearly this situation is not physically realized. The way out of the seeming paradox is the spontaneous symmetry breaking of the collective system.¹ The description of spontaneous symmetry breaking in macroscopic systems that are constructed from microscopic, quantum mechanical constituents is one of the highlights of condensed matter theory.^{2–6} It is used to explain the classical features of macroscopic systems ranging from crystals and antiferromagnets to superconductors.⁷

The general idea behind spontaneous symmetry breaking is easily formulated: as a collection of quantum particles becomes larger, the symmetry of the system as a whole becomes more unstable against small perturbations. In the limit of an infinite system an infinitesimal perturbation is enough to cause the system to break the underlying symmetry of the Hamiltonian. The fact that the symmetry breaking can happen spontaneously is signaled by a set of noncommuting limits: In the complete absence of perturbations even a macroscopic system should conform to the symmetry of the Hamiltonian. However, in the presence of an infinitesimal perturbation a macroscopic system will be able to break the symmetry and end up in a classical state. This intuitive picture of spontaneous symmetry breaking is not always easy to demonstrate in an equally clear mathematical description of the process.

In this paper we present a simple mathematical procedure that can be applied to the spontaneous breaking of any continuous symmetry and that naturally emphasizes the roles of the key players (the symmetry-breaking field, the thermodynamic limit, and the global excitations of a “thin” spectrum) in this symmetry breaking. The procedure is described by considering the example of a quantum harmonic crystal that spontaneously breaks translational symmetry. All of the methods, that is, bosonization, using the Bogoliubov transformation to identify the “thin” spectrum of states involved in spontaneous symmetry breaking, introducing a symmetry-

breaking field in the collective dynamics, and considering a noncommuting order of limits, can be applied to other systems as well.^{8–10}

II. THE HARMONIC CRYSTAL

As a basic example of spontaneous symmetry breaking, we consider how translational symmetry is broken in a crystalline lattice.⁹ Consider a harmonic crystal with the Hamiltonian

$$H = \sum_j \frac{p_j^2}{2m} + \frac{\kappa}{2} \sum_j (x_j - x_{j+1})^2, \quad (1)$$

where j labels the N atoms in the lattice, which have mass m , momentum p_j , and position x_j . We consider here only a one-dimensional chain of atoms, but all of the following can be straightforwardly generalized to higher dimensions. The parameter κ gives the strength of the harmonic potential between neighboring atoms. The results on spontaneous symmetry breaking that follow are equally valid for anharmonic potentials.⁹

In the standard treatment of the harmonic oscillator a Fourier transformation of the Hamiltonian is used to identify its eigenstates. We follow a slightly longer route by introducing boson (phonon) operators from the outset and diagonalizing them using the Bogoliubov transformation.¹¹ This approach has the advantages that it naturally brings to the fore the thin spectrum of the crystal and enables us to keep track of the center of mass motion of the crystal as a whole.¹² The momentum and position operators can be expressed in terms of boson operators as

$$p_j = iC \sqrt{\frac{\hbar}{2}} (b_j^\dagger - b_j), \quad (2)$$

$$x_j = \frac{1}{C} \sqrt{\frac{\hbar}{2}} (b_j^\dagger + b_j), \quad (3)$$

so that the commutation relation $[x_j, p_{j'}] = i\hbar \delta_{j,j'}$ is satisfied. We choose $C^2 = \sqrt{2m\kappa}$ so that the Hamiltonian reduces to

$$H = \frac{\hbar}{4} \sqrt{\frac{2\kappa}{m}} \sum_j [2(b_j^\dagger b_j + b_j b_j^\dagger) - (b_j^\dagger + b_j)(b_{j+1}^\dagger + b_{j+1})]. \quad (4)$$

After a Fourier transformation we have

$$H = \sqrt{\frac{\hbar^2 \kappa}{2m}} \sum_k \left[A_k b_k^\dagger b_k + \frac{B_k}{2} (b_k^\dagger b_{-k}^\dagger + b_k b_{-k}) + 1 \right], \quad (5)$$

where $A_k = 2 - \cos(ka)$, $B_k = -\cos(ka)$, and a is the lattice constant. This Hamiltonian is still not diagonal, because the terms $b_k^\dagger b_{-k}^\dagger$ and $b_k b_{-k}$ create and annihilate two bosons at the same time. We get rid of these terms by introducing transformed operators $\beta_k = \cosh(u_k) b_{-k} + \sinh(u_k) b_k^\dagger$ and choosing u_k such that the resulting Hamiltonian is diagonal. After this Bogoliubov transformation, the Hamiltonian in terms of transformed bosons is given by

$$H = \hbar \sqrt{\frac{\kappa}{m}} \sum_k \left[2 \sin \left| \frac{ka}{2} \right| \left(\beta_k^\dagger \beta_k + \frac{1}{2} \right) + \frac{1}{4} \sqrt{2} \cos(ka) \right] \quad (6a)$$

$$= 2\hbar \sqrt{\frac{\kappa}{m}} \sum_k \sin \left| \frac{ka}{2} \right| \left[n_k + \frac{1}{2} \right], \quad (6b)$$

because $\sum_k \cos k = (N/2\pi) \int_{-\pi}^{\pi} dk \cos k = 0$.

III. THE THIN SPECTRUM

The form (6b) of the Hamiltonian in terms of phonon operators coincides with the standard textbook result.¹³ The use of the Bogoliubov transformation to obtain Eq. (6b) has the advantage that it draws attention to a rather subtle point. When $k \rightarrow 0$ the excitation energy $\omega_k \rightarrow 0$, and the two parameters in the Bogoliubov transformation diverge [$\sinh(u_k) \rightarrow \infty$ and $\cosh(u_k) \rightarrow \infty$]. Thus at $k=0$ the canonical transformation is no longer well defined, and we should treat the $k=0$ part of the Hamiltonian (1) separately from the rest.¹² The excitations with $k=0$ are the ones that describe the collective dynamics of the crystal as a whole, and therefore they are also the states that are involved in the collective symmetry breaking. The $k=0$ part of the Hamiltonian, written in terms of the original operators, is given by

$$H_{\text{coll}} = \frac{p_{\text{tot}}^2}{2Nm} + \text{const}, \quad (7)$$

where $p_{\text{tot}} \equiv \sum_j p_j = \sqrt{N} p_{k=0}$ is the total momentum of the system. It can easily be checked that this part of the Hamiltonian, which describes the external dynamics of the crystal as a whole, commutes with the rest of the Hamiltonian, which describes the internal dynamics of the phonon modes inside the crystal. We therefore focus on the collective part of the Hamiltonian and disregard the phonon spectrum given by Eq. (6b).

Notice that by considering only the collective part of the Hamiltonian, we have effectively reduced the problem to a single-particle problem. The single particle in Eq. (7) with mass Nm and momentum p_{tot} describes the dynamics of the crystal as a whole. Its momentum and position are the center of mass momentum and position of the crystal. In contrast, Eq. (6b) describes the internal degrees of freedom of the crystal and includes all many-body effects that arise from the coupling of the N individual atoms.

The relevant eigenstates of the collective Hamiltonian (7) are very low in energy: their excitation energies scale as $1/N$, where N is the number of atoms in the crystal.¹⁴ In the thermodynamic limit all of these states thus become nearly degenerate. Because of this property a combination of these

states that break the symmetry of the Hamiltonian can be spontaneously formed in the thermodynamic limit. At the same time, these collective eigenstates are so few in number and of such low energy that their contribution to the free energy completely disappears in the thermodynamic limit. This vanishing contribution can be seen by looking at their contribution to the partition function

$$Z_{\text{thin}} = \sum e^{-\beta H_{\text{coll}}} \propto \sqrt{N}, \quad (8a)$$

$$F_{\text{thin}} = -T \ln(Z_{\text{thin}}) \propto \ln(N). \quad (8b)$$

The free energy of the total system is an extensive quantity, so that $F_{\text{thin}}/F_{\text{tot}} \propto \ln(N)/N$ disappears in the limit $N \rightarrow \infty$. The states of this part of the spectrum are thus invisible in thermodynamically measurable quantities such as for instance the specific heat of macroscopic crystals, and it is consequently called the *thin spectrum* of the quantum crystal.

To see how the states in the thin spectrum can conspire to break the translational symmetry, we need to add a small symmetry-breaking field to the Hamiltonian:

$$H_{\text{coll}}^{\text{SB}} = \frac{p_{\text{tot}}^2}{2Nm} + \frac{B}{2} x_{\text{tot}}^2. \quad (9)$$

Here the symmetry-breaking field B is introduced as a mathematical tool and need not actually exist. We will send the value of B to zero at the end of the calculation. The Hamiltonian (9) is the standard form of the Hamiltonian for a quantum harmonic oscillator, and its eigenstates are well known. The ground state wavefunction can be written as

$$\psi_0(x_{\text{tot}}) = \left(\frac{m\omega N}{\pi \hbar} \right)^{1/4} e^{-(m\omega N/2\hbar)x_{\text{tot}}^2}, \quad (10)$$

with $\omega = \sqrt{B/mN}$. This ground state is a wavepacket of the total momentum states that make up the thin spectrum. Apart from the ground state configuration there are also collective eigenstates that are described by the excitations of the harmonic oscillator Eq. (9). These excitations describe the collective motion of the crystal as a whole. As N becomes larger, the ground state wavepacket becomes more and more localized at the position $x_{\text{tot}}=0$, until it is completely localized as $N \rightarrow \infty$. That this localization can occur spontaneously without the existence of a physical symmetry-breaking field B can be seen by considering the noncommuting limits

$$\lim_{N \rightarrow \infty} \lim_{B \rightarrow 0} |\psi_0(x_{\text{tot}})|^2 = \text{const}, \quad (11)$$

$$\lim_{B \rightarrow 0} \lim_{N \rightarrow \infty} |\psi_0(x_{\text{tot}})|^2 = \delta(x_{\text{tot}}). \quad (12)$$

If we do not include any symmetry-breaking field, then the crystal is always completely delocalized and respects the symmetry of the Hamiltonian.¹⁵ If we do allow for a symmetry-breaking field, then it turns out that in the limit of having infinitely many constituent particles, an infinitesimally small symmetry-breaking field is enough to completely localize the crystal at a single position. This mathematical instability implies that the symmetry breaking happens spontaneously in the thermodynamic limit.

Notice that once the crystal has been localized at a specific position and the unphysical symmetry-breaking field has

been sent to zero, the delocalization of the crystal due to the spreading of its wavefunction will take a time proportional to N and can thus never be observed.

To see more rigorously whether or not the crystal as a whole is localized, we should look at the spatial fluctuations of the crystal $\langle x_{\text{tot}}^2 \rangle$. The absolute size of these fluctuations by itself is meaningless. Their size becomes meaningful only if it is compared to the size of the crystal. Because the size of the crystal is proportional to the number of particles in the system, the appropriate order parameter in this case is $\langle x_{\text{tot}}^2 \rangle/N$. This order parameter has a noncommuting order of limits as $N \rightarrow \infty$,

$$\lim_{N \rightarrow \infty} \lim_{B \rightarrow 0} \langle x_{\text{tot}}^2 \rangle/N = \infty, \quad (13)$$

$$\lim_{B \rightarrow 0} \lim_{N \rightarrow \infty} \langle x_{\text{tot}}^2 \rangle/N = 0, \quad (14)$$

which again signals the spontaneous localization of the crystal as a whole.

IV. SUBTLETIES

In the derivation of the spontaneous symmetry breaking of a harmonic crystal we have been somewhat sloppy in the definition of the symmetry-breaking field. After all, the collective model of Eq. (7) was only the $k=0$ part of the full blown Hamiltonian in Eq. (1), but we did not consider the symmetry-breaking field to be only the $k=0$ part of some other field acting on all atoms individually. It would therefore be better to start with a microscopic model, which already includes a symmetry-breaking field such as

$$H^{\text{SB}} = \sum_j \left[\frac{p_j^2}{2m} + \frac{\kappa}{2} (x_j - x_{j+1})^2 + B(1 - \cos(x_j)) \right] \quad (15)$$

$$\rightarrow H_{\text{coll}}^{\text{SB}} \simeq \frac{p_{\text{tot}}^2}{2Nm} + \frac{B}{2N} x_{\text{tot}}^2. \quad (16)$$

In Eq. (16) we again consider only the $k=0$ part of the Hamiltonian and have expanded the cosine to quadratic order. The fact that the symmetry-breaking field now scales as $1/N$ is a direct consequence of our definition of the microscopic symmetry-breaking field. The factor $1/N$ cannot be avoided if we insist that the microscopic Hamiltonian be extensive. This factor might seem to imply an end to the localization of the total wavefunction $\psi_0(x_{\text{tot}})$, but spontaneous symmetry breaking is still possible as long as we consider the correct order parameter. Even though the wavefunction itself does not reduce to a Dirac delta function anymore, the spatial fluctuations of the crystal compared to its size still become negligible in the thermodynamic limit if an infinitesimal symmetry-breaking field is included:

$$\lim_{N \rightarrow \infty} \lim_{B \rightarrow 0} \langle x_{\text{tot}}^2 \rangle/N = \infty, \quad (17)$$

$$\lim_{B \rightarrow 0} \lim_{N \rightarrow \infty} \langle x_{\text{tot}}^2 \rangle/N = 0. \quad (18)$$

Once again the disappearance of fluctuations in the thermodynamic limit signals the spontaneous localization of the crystal as a whole.

This digression into extensivity and the correct choice for the symmetry-breaking field seems unnecessary for under-

standing the essential ingredients of spontaneous symmetry breaking, and therefore we have ignored these subtleties in our main treatment of quantum spontaneous symmetry breaking. In the application of this procedure to other systems, such as antiferromagnets and superconductors, these issues don't arise because we are forced to consider extensive models from the outset. In these cases, however, the mathematics of diagonalizing the collective Hamiltonian is a bit more involved.^{9,10}

V. DISCUSSION

We have presented a simple way of explaining the appearance of spontaneous symmetry breaking in quantum systems. The procedure starts with the bosonization of the microscopic Hamiltonian. The quadratic part of the bosonized Hamiltonian can in principle be diagonalized using a Bogoliubov transformation, but in doing so we find that there are some modes for which the transformation is ill-defined. These singular modes are the ones that describe the dynamics of the system as a whole (in contrast to the dynamics of constituent particles within the system). These collective excitations should be treated separately from all other modes, and together they define the collective part of the Hamiltonian of the system. The eigenstates of this collective Hamiltonian that scale as $1/N$ form the thin spectrum. It is a combination of these states that make up the symmetry broken wavefunction. As a mathematical tool necessary to be able to see the symmetry breaking explicitly, we introduced the symmetry-breaking field B . If we look at the new ground state wavefunction or at a suitably defined order parameter for the system, we see that in the thermodynamic limit an infinitesimally small field B is enough to completely break the symmetry of the underlying Hamiltonian. It is thus argued that symmetry breaking can happen spontaneously in the limit $N \rightarrow \infty$.

The method as presented here can be adapted to describe rotors, antiferromagnets, and even superconductors, and should in principle be applicable to all quantum systems that spontaneously break some continuous symmetry.

VI. PROBLEMS

- (1) Check that the thin spectrum of a harmonic crystal is indeed "thin." That is,
 - (a) Show that only the lowest \sqrt{N} total momentum states are not exponentially suppressed in the symmetry broken wavefunction (10). (This result implies that only the lowest \sqrt{N} total momentum states contribute to the symmetry broken wavefunction, and these states all become degenerate in the thermodynamic limit.)
 - (b) Calculate the partition function of the thin spectrum states and show that it scales as \sqrt{N} , so that the contribution of these states to the free energy vanishes in the thermodynamic limit.
- (2) Show the noncommutativity of the limits in Eq. (14) explicitly, by going through the following steps:
 - (b) Formulate the Hamiltonian of Eq. (9) in terms of the boson (raising and lowering) operators $b^\dagger = \sqrt{C/(2\hbar)} \times (x_{\text{tot}} - i/Cp_{\text{tot}})$ and $b = \sqrt{C/(2\hbar)}(x_{\text{tot}} + i/Cp_{\text{tot}})$ (where C is some constant).
 - (c) Choose C such that the Hamiltonian becomes diagonal and find its ground state.

- (d) Evaluate the limits of Eq. (14) by expressing x_{tot}^2 in terms of boson operators and taking the expectation value with respect to the ground state of $H_{\text{coll}}^{\text{SB}}$.
- (3) Work out the Bogoliubov transformation of Eqs. (5) and (6b) explicitly.
- (a) Write the Hamiltonian of Eq. (5) in terms of the transformed bosons $\beta_k = \cosh(u_k)b_{-k} + \sinh(u_k)b_k^\dagger$.
- (b) Which value should be chosen for u_k in order for the Bogoliubov transformation to yield the diagonal Hamiltonian of Eq. (6b)? [Answer: $\tanh(2u_k) = B_k/A_k$.]

¹ Although the mechanism of spontaneous symmetry breaking presented in this paper is generally accepted as the mechanism responsible for the occurrence of asymmetric states in quantum systems in the thermodynamic limit and is used to explain effects in subfields of physics ranging from high energy physics to condensed matter theory and cosmology, some alternative views on the workings of symmetry breaking exist. See M. Simonius, "Spontaneous symmetry breaking and blocking of metastable states," *Phys. Rev. Lett.* **40**, 980–983 (1978); M. Tegmark, "Parallel universes," in *Science and Ultimate Reality*, edited by J. D. Barrow, P. C. Davies, and C. L. Harper (Cambridge U. P., Cambridge, 2004), pp. 459–491; O. Dreyer, "Emergent probabilities in quantum mechanics," *quant-ph/0603202* (2006).

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⁷ Notice that ferromagnetism is explicitly not included in this list. The ferromagnet has a large number of possible exact ground states that are precisely degenerate and all have a finite magnetization. The singling out of one of these eigenstates is more like classical symmetry breaking than like the quantum symmetry breaking discussed here. Quantum symmetry breaking causes a state that is not an eigenstate of the Hamiltonian to be realized, and thus goes much further than singling out only one particular eigenstate.

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¹¹ See, for example, Ph. A. Martin and F. Rothen, *Many-Body Problems and Quantum Field Theory, An Introduction* (Springer-Verlag, Berlin, 2002), pp. 218 and 254–258.

¹² See, for example, Ref. 11, pp. 42–48.

¹³ See, for example, P. L. Taylor and O. Heinonen, *A Quantum Approach to Condensed Matter Physics* (Cambridge U. P., Cambridge, 2002), pp. 93–99.

¹⁴ This argument holds only for the lowest \sqrt{N} eigenstates. As can be seen from Eq. (10), these are the only states contributing to the symmetry-broken ground state, as all other states are exponentially suppressed.

¹⁵ Note that the wavefunction in Eq. (12) is not properly normalized due only to the non-normalizability of the free-particle wavefunction in quantum mechanics. This non-normalizability can be cured in the usual way by introducing a finite space and periodic boundary conditions. By letting the size of the space tend to infinity, the properties of the free particle in infinite space are recovered.