

## BOGOLIUBOV'S VISION: QUASIAVERAGES AND BROKEN SYMMETRY TO QUANTUM PROTECTORATE AND EMERGENCE

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In the present interdisciplinary review, we focus on the applications of the symmetry principles to quantum and statistical physics in connection with some other branches of science. The profound and innovative idea of quasiaverages formulated by N. N. Bogoliubov, gives the so-called macro-objectivation of the degeneracy in the domain of quantum statistical mechanics, quantum field theory and quantum physics in general. We discuss the complementary unifying ideas of modern physics, namely: spontaneous symmetry breaking, quantum protectorate and emergence. The interrelation of the concepts of symmetry breaking, quasiaverages and quantum protectorate was analyzed in the context of quantum theory and statistical physics. The chief purposes of this paper were to demonstrate the connection and interrelation of these conceptual advances of the many-body physics and to try to show explicitly that those concepts, though different in details, have certain common features. Several problems in the field of statistical physics of complex materials and systems (e.g., the chirality of molecules) and the foundations of the microscopic theory of magnetism and superconductivity were discussed in relation to these ideas.

*Keywords:* Symmetry principles; the breaking of symmetries; statistical physics and condensed matter physics; quasiaverages; Bogoliubov's inequality; quantum protectorate; emergence; chirality; quantum theory of magnetism; theory of superconductivity.

### 1. Introduction

There have been many interesting and important developments in statistical physics during the past decades. It is well-known that symmetry principles play a crucial role in physics.<sup>1–8</sup> The theory of symmetry is a basic tool for understanding and formulating the fundamental notions of physics.<sup>9,10</sup> Symmetry considerations show that symmetry arguments are very powerful tools for bringing order into the very complicated picture of the real world.<sup>11–14</sup> As was rightly noticed by R. L. Mills, “symmetry is a driving force in the shaping of physical theory”.<sup>15</sup> According to D. Gross, “the primary lesson of physics of this century is that the secret of nature

is symmetry".<sup>16</sup> Every symmetry leads to a conservation law<sup>17–19</sup>; the well-known examples are the conservation of energy, momentum and electrical charge. A variety of other conservation laws can be deduced from symmetry or invariance properties of the corresponding Lagrangian or Hamiltonian of the system. According to Noether theorem, every continuous symmetry transformation under which the Lagrangian of a given system remains invariant implies the existence of a conserved function.<sup>8,13</sup>

Many fundamental laws of physics in addition to their detailed features possess various symmetry properties. These symmetry properties lead to certain constraints and regularities on the possible properties of matter. Thus the principles of symmetries belong to the **underlying principles** of physics. Moreover, the idea of symmetry is a useful and workable tool for many areas of the quantum field theory, statistical physics and condensed matter physics.<sup>14,20–23</sup> However, it is worth stressing the fact that all symmetry principles have an empirical basis.

The invariance principles of nonrelativistic quantum mechanics<sup>17,18,24–27</sup> include those associated with space translations, space inversions, space rotations, Galilean transformations, and time reversal. In relation to these transformations, the important problem was to give a presentation in terms of the properties of the dynamical equations under appropriate coordinate transformations and to establish the relationship to certain contact transformations.

The developments in many-body theory and quantum field theory, in the theory of phase transitions, and in the general theory of symmetry provided a new perspective. As was emphasized by Callen,<sup>28,29</sup> it appeared that symmetry considerations lie ubiquitously at the very roots of thermodynamic theory, so universally and so fundamentally that they suggest a new conceptual basis. The interpretation proposed by Callen<sup>28,29</sup> suggests that thermodynamics is the study of those properties of macroscopic matter that follow from the symmetry properties of physical laws, mediated through the statistics of large systems.

In the many body problem and statistical mechanics, one studies systems with infinitely many degrees of freedom. Since actual systems are finite but large, it means that one studies a model which is not only mathematically simpler than the actual system, but also allows a more precise formulation of phenomena such as phase transitions, transport processes, which are typical for macroscopic systems. States not invariant under symmetries of the Hamiltonian are of importance in many fields of physics.<sup>30–33</sup> In principle, it is necessary to clarify and generalize the notion of state of a system,<sup>34,35</sup> depending on the algebra of observables  $\mathcal{U}$ . In the case of truly finite system, the normal states are the most general states. However, all states in statistical mechanics are of the more general states.<sup>35</sup> From this point of view, a study of the automorphisms of  $\mathcal{U}$  is of significance for a classification of states.<sup>35</sup> In other words, the transformation  $\Psi(\eta) \rightarrow \Psi(\eta) \exp(i\alpha)$  for all  $\eta$  leaves the commutation relations invariant. Gauge transformation define a one-parameter group of automorphisms. In most cases, the three group of transformations, namely translation in space, evolution in time and gauge transformation, commute with

each other. Due to the quasi-local character of the observables, one can prove that<sup>35</sup>

$$\lim_{|x| \rightarrow \infty} \|[A_{\mathbf{x}}, B]\| = 0.$$

It is possible to say therefore that the algebra  $\mathcal{U}$  of observables is asymptotically Abelian for space translation. A state which is invariant with respect to translations in space and time, we can call respectively homogeneous and stationary. If a state is invariant for gauge transformation, we say that the state has a fixed particle number.

In physics, spontaneous symmetry breaking occurs when a system that is symmetric with respect to some symmetry group goes into a vacuum state that is not symmetric. When that happens, the system no longer appears to behave in a symmetric manner. It is a phenomenon that naturally occurs in many situations. The symmetry group can be discrete, such as the space group of a crystal, or continuous (e.g., a Lie group), such as the rotational symmetry of space.<sup>11–14</sup> However, if the system contains only a single spatial dimension, then only discrete symmetries may be broken in a vacuum state of the full quantum theory, although a classical solution may break a continuous symmetry. The problem of great importance is to understand the domain of validity of the broken symmetry concept.<sup>32,33</sup> It is of significance to understand whether it is valid only at low energies (temperatures), or whether it is universally applicable.<sup>36</sup>

Symmetries and breaking of symmetries play an important role in statistical physics,<sup>37–44</sup> classical mechanics,<sup>41–45</sup> condensed matter physics<sup>46–48</sup> and particle physics.<sup>24,25,49–54</sup> Symmetry is a crucial concept in the theories that describe the subatomic world<sup>30,31</sup> because it has an intimate connection with the laws of conservation. For example, the fact that physics is invariant everywhere in the universe means that linear momentum is conserved. Some symmetries, such as rotational invariance, are perfect. Others, such as parity, are broken by small amounts, and the corresponding conservation law therefore only holds approximately.

In particle physics, the natural question sounds as what is it that determines the mass of a given particle and how is this mass related to the mass of other particles.<sup>55</sup> The partial answer to this question has been given within the frame work of a broken symmetry concept. For example, in order to describe properly the  $SU(2) \times U(1)$  theory in terms of electroweak interactions, it is necessary to deduce how massive gauge quanta can emerge from a gauge-invariant theory. To resolve this problem, the idea of spontaneous symmetry breaking was used.<sup>48,49,54</sup> From the other hand, the application of the Ward identities reflecting the  $U(1)_{\text{em}} \times SU(2)_{\text{spin}}$ -gauge invariance of non-relativistic quantum mechanics<sup>26</sup> leads to a variety of generalized quantized Hall effects.<sup>56,57</sup>

The mechanism of spontaneous symmetry breaking is usually understood as the mechanism responsible for the occurrence of asymmetric states in quantum systems in the thermodynamic limit and is used in various fields of quantum physics. However, the broken symmetry concept can be used as well in classical physics.<sup>58</sup>

It was shown in Ref. 59 that starting from a standard description of an ideal, isentropic fluid, it was possible to derive the effective theory governing a gapless non-relativistic mode — the sound mode. The theory, which was dictated by the requirement of Galilean invariance, entails the entire set of hydrodynamic equations. The gaplessness of the sound mode was explained by identifying it as the Goldstone mode associated with the spontaneous breakdown of the Galilean invariance. Thus the presence of sound waves in an isentropic fluid was explained as an *emergent property*.

It is appropriate to note here that the emergent properties of matter were analyzed and discussed by R. Laughlin and D. Pines<sup>60,61</sup> from a general point of view (see also Ref. 62). They introduced a unifying idea of *quantum protectorate*. This concept belongs also to the underlying principles of physics. The idea of quantum protectorate reveals the essential difference in the behavior of the complex many-body systems at the low-energy and high-energy scales. The existence of two scales, low-energy and high-energy, in the description of physical phenomena is used in physics, explicitly or implicitly. It is worth noting that standard thermodynamics and statistical mechanics are intended to describe the properties of many-particle system at low energies, like the temperature and pressure of the gas. For example, it was known for many years that a system in the low-energy limit can be characterized by a small set of “collective” (or hydrodynamic) variables and equations of motion corresponding to these variables. Going beyond the framework of the low-energy region would require the consideration of high-energy excitations.

It should be stressed that symmetry implies degeneracy. The greater the symmetry, the greater the degeneracy. The study of the degeneracy of the energy levels plays a very important role in quantum physics. There is an additional aspect of the degeneracy problem in quantum mechanics, when a system possesses more subtle symmetries. This is the case when degeneracy of the levels arises from the invariance of the Hamiltonian  $H$  under groups involving simultaneous transformation of coordinates and momenta that contain as subgroups the usual geometrical groups based on point transformations of the coordinates. For these groups, the free part of  $H$  is not invariant, so that the symmetry is established only for interacting systems. For this reason, they are usually called dynamical groups. Particular case is the hydrogen atom,<sup>63–65</sup> whose so-called *accidental degeneracy* of the levels of given principal quantum number is due to the symmetry of  $H$  under the four-dimensional rotation group  $O(4)$ .

It is of importance to emphasize that when spontaneous symmetry breaking takes place, the ground state of the system is degenerate. Substantial progress in the understanding of the spontaneously broken symmetry concept is connected with Bogoliubov’s fundamental ideas about quasiaverages.<sup>37,66–68</sup> Studies of degenerated systems led Bogoliubov in 1960–61 to the formulation of **the method of quasiaverages**. This method has proved to be a universal tool for systems whose ground states become unstable under small perturbations. Thus the role of symmetry (and the breaking of symmetries) in combination with the degeneracy of the system was

reanalyzed and essentially clarified by N. N. Bogoliubov in 1960–1961. He invented and formulated a powerful innovative idea of *quasiaverages* in statistical mechanics.<sup>37,66–68</sup> The very elegant work of N. N. Bogoliubov on *quasiaverages*<sup>66</sup> has been of great importance for a deeper understanding of phase transitions, superfluidity and superconductivity, magnetism and other fields of equilibrium and nonequilibrium statistical mechanics.<sup>37,66–70</sup> Bogoliubov's idea of *quasiaverages* is an essential conceptual advance of modern physics.

According to F. Wilczek,<sup>71</sup> “the primary goal of fundamental physics is to discover profound concepts that illuminate our understanding of nature”. The chief purposes of this paper are to demonstrate the connection and interrelation of three conceptual advances (or “profound concepts”) of the many-body physics, namely the broken symmetry, quasiaverages and quantum protectorate, and to try to show explicitly that those concepts, though different in details, have certain common features.

## 2. Gauge Invariance

An important class of symmetries is the so-called dynamical symmetry. The symmetry of electromagnetic equation under gauge transformation can be considered as a prototype of the class of dynamical symmetries.<sup>51</sup> The conserved quantity corresponding to gauge symmetry is the electric charge. A gauge transformation is a unitary transformation  $U$  which produces a local phase change

$$U\phi(x) \rightarrow e^{i\Lambda(x)}\phi(x), \quad (2.1)$$

where  $\phi(x)$  is the classical local field describing a charged particle at point  $x$ . The phase factor  $e^{i\Lambda(x)}$  is the representation of the one-dimensional unitary group  $U(1)$ .

F. Wilczek pointed out that “gauge theories lie at the heart of modern formulation of the fundamental laws of physics. The special characteristic of these theories is their extraordinary degree of symmetry, known as gauge symmetry or gauge invariance”.<sup>72</sup>

The usual gauge transformation has the form

$$A_\mu \rightarrow A'_\mu - (\partial/\partial x^\mu)\lambda, \quad (2.2)$$

where  $\lambda$  is an arbitrary differentiable function from space-time to the real numbers,  $\mu$  being 1, 2, 3, or 4. If every component of  $A$  is changed in this fashion, the  $\vec{E}$  and  $\vec{B}$  vectors, which by Maxwell equations characterize the electromagnetic field, are left unaltered, so therefore the field described by  $A$  is equally well-characterized by  $A'$

Few conceptual advances in theoretical physics have been as exciting and influential as gauge invariance.<sup>73,74</sup> Historically, the definition of gauge invariance was originally introduced in the Maxwell theory of electromagnetic field.<sup>51,75,76</sup> The introduction of potentials is a common procedure in dealing with problems in electrodynamics. In this way, Maxwell equations were rewritten in forms which are

rather simple and more appropriate for analysis. In this theory, common choices of gauge are  $\vec{\nabla} \cdot \vec{A} = 0$ , called the Coulomb gauge. There are many other gauges. In general, it is necessary to select the scalar gauge function  $\chi(x, t)$  whose spatial and temporal derivatives transform one set of electromagnetic potential into another equivalent set. A violation of gauge invariance means that there are some parts of the potentials that do not cancel. For example, Yang and Kobe<sup>77</sup> have used the gauge dependence of the conventional interaction Hamiltonian to show that the conventional interpretation of the quantum mechanical probabilities violates causality in those gauges with advanced potentials or faster-than- $c$  retarded potentials.<sup>78,79</sup> Significance of electromagnetic potentials in the quantum theory was demonstrated by Aharonov and Bohm<sup>80</sup> in 1959 (see also Ref. 81).

The gauge principle implies an invariance under internal symmetries performed independently at different points of space and time.<sup>82</sup> The known example of gauge invariance is a change in phase of the Schrödinger wave function for an electron

$$\Psi(x, t) \rightarrow e^{iq\varphi(x,t)/\hbar}\Psi(x, t) \quad (2.3)$$

In general, in quantum mechanics the wave function is complex, with a phase factor  $\varphi(x, t)$ . The phase change varies from point to point in space and time. It is well-known<sup>56,57</sup> that such phase changes form a  $U(1)$  group at each point of space and time, called the gauge group. The constant  $q$  in the phase change is the electric charge of the electron. It should be emphasized that not all theories of the gauge type can be internally consistent when quantum mechanics is fully taken into account.

Thus the gauge principle, which might also be described as a principle of local symmetry, is a statement about the invariance properties of physical laws. It requires that every continuous symmetry is a local symmetry. The concepts of local and global symmetry are highly non-trivial. The operation of global symmetry acts simultaneously on all variables of a system whereas the operation of local symmetry acts independently on each variable. Two known examples of phenomena that are indeed associated with local symmetries are electromagnetism (where we have a local  $U(1)$  invariance), and gravity (where the group of Lorentz transformations is replaced by general, local coordinate transformations). According to D. Gross,<sup>16</sup> “there is an essential difference between gauge invariance and global symmetry such as translation or rotational invariance. Global symmetries are symmetries of the laws of nature . . . we search now for a synthesis of these two forms of symmetry [local and global], a unified theory that contains both as a consequence of a greater and deeper symmetry, of which these are the low energy remnants . . .”.

There is the general Elitzur’s theorem,<sup>83</sup> which states that a spontaneous breaking of local symmetry for symmetrical gauge theory without gauge fixing is impossible. In other words, local symmetry can never be broken and a non gauge invariant quantity never acquires nonzero vacuum expectation value. This theorem was analyzed and refined in many papers.<sup>84,85</sup> K. Splitdorff<sup>85</sup> analyzed the impossibility of spontaneously breaking local symmetries and the sign problem. Elitzur’s theorem

stating the impossibility of spontaneous breaking of local symmetries in a gauge theory was reexamined. The existing proofs of this theorem rely on gauge invariance as well as positivity of the weight in the Euclidean partition function. Splittorff examined the validity of Elitzur's theorem in gauge theories for which the Euclidean measure of the partition function is not positive definite. He found that Elitzur's theorem does not follow from gauge invariance alone. A general criterion under which spontaneous breaking of local symmetries in a gauge theory is excluded was formulated.

Quantum field theory and the principle of gauge symmetry provide a theoretical framework for constructing effective models of systems consisting of many particles<sup>86</sup> and condensed matter physics problems.<sup>87</sup> It was also shown recently<sup>88</sup> that the gauge symmetry principle inherent in Maxwell's electromagnetic theory can be used in the efforts to reformulate general relativity into a gauge field theory. The gauge symmetry principle has been applied in various forms to quantize gravity.

Popular unified theories of weak and electromagnetic interactions are based on the notion of a spontaneously broken gauge symmetry. The hope has also been expressed by several authors that suitable generalizations of such theories may account for strong interactions as well. It was conjectured that the spontaneous breakdown of gauge symmetries may have a cosmological origin. As a consequence, it was proposed that at some early stage of development of an expanding universe, a phase transition takes place. Before the phase transition, weak and electromagnetic interactions (and perhaps strong interactions too) were of comparable strengths. The presently observed differences in the strengths of the various interactions develop only after the phase transition takes place.

To summarize, the following sentence of D. Gross is appropriate for the case: "the most advanced form of symmetries we have understood are local symmetries — general coordinate invariance and gauge symmetry. In contrast, we do not believe that global symmetries are fundamental. Most global symmetries are approximate and even those that, so far, have shown no sign of been broken, like baryon number and perhaps *CPT*, are likely to be broken. They seem to be simply accidental features of low energy physics. Gauge symmetry, however, is never really broken — it is only hidden by the asymmetric macroscopic state we live in. At high temperature or pressure, gauge symmetry will always be restored".<sup>16</sup>

### 3. Spontaneous Symmetry Breaking

As it was mentioned earlier, a symmetry can be exact or approximate.<sup>30,32,33</sup> Symmetries inherent in the physical laws may be dynamically and spontaneously broken, i.e., they may not manifest themselves in the actual phenomena. It can be as well broken by certain reasons. C. N. Yang<sup>89</sup> pointed out, that non-Abelian gauge field become very useful in the second half of the twentieth century in the unified theory of electromagnetic and weak interactions, combined with symmetry breaking. Within the literature the term *broken symmetry* is used both very often and with

different meanings. There are two terms, the spontaneous breakdown of symmetries and dynamical symmetry breaking,<sup>90</sup> which sometimes have been used as opposed but such a distinction is irrelevant. According to Y. Nambu,<sup>49</sup> the two terms may be used interchangeably. As it was mentioned previously, a symmetry implies degeneracy. In general, there are a multiplets of equivalent states related to each other by congruence operations. They can be distinguished only relative to a weakly coupled external environment which breaks the symmetry. Local gauged symmetries, however, cannot be broken this way because such an extended environment is not allowed (a superselection rule), so all states are singlets, i.e., the multiplicities are not observable except possibly for their global part. In other words, since a symmetry implies degeneracy of energy eigenstates, each multiplet of states forms a representation of a symmetry group  $G$ . Each member of a multiple is labeled by a set of quantum numbers for which one may use the generators and Casimir invariants of the chain of subgroups, or else some observables which form a representation of  $G$ . It is a dynamical question whether or not the ground state, or the most stable state, is a singlet, a most symmetrical one.<sup>49</sup>

Peierls<sup>32,33</sup> gives a general definition of the notion of the spontaneous breakdown of symmetries which is suited equally well for the physics of particles and condensed matter physics. According to Peierls,<sup>32,33</sup> the term *broken symmetries* relates to situations in which symmetries which we expect to hold are valid only approximately or fail completely in certain situations.

The intriguing mechanism of spontaneous symmetry breaking is a unifying concept that lie at the basis of most of the recent developments in theoretical physics, from statistical mechanics to many-body theory and to elementary particles theory. It is known that when the Hamiltonian of a system is invariant under a symmetry operation, but the ground state is not, the symmetry of the system can be spontaneously broken.<sup>13</sup> Symmetry breaking is termed *spontaneous* when there is no explicit term in a Lagrangian which manifestly breaks the symmetry.<sup>91-93</sup>

The existence of degeneracy in the energy states of a quantal system is related to the invariance or symmetry properties of the system. By applying the symmetry operation to the ground state, one can transform it to a different but equivalent ground state. Thus the ground state is degenerate, and in the case of a continuous symmetry, infinitely degenerate. The real, or relevant, ground state of the system can only be one of these degenerate states. A system may exhibit the full symmetry of its Lagrangian, but it is characteristic of infinitely large systems that they also may condense into states of lower symmetry. According to Anderson,<sup>94</sup> this leads to an essential difference between infinite systems and finite systems. For infinitely extended systems, a symmetric Hamiltonian can account for non symmetric behaviors, giving rise to non symmetric realizations of a physical system.

In terms of group theory,<sup>13,95,96</sup> it can be formulated that if for a specific problem in physics, we can write down a basic set of equations which is invariant under a certain symmetry group  $G$ , then we would expect that solutions of these equations would reflect the full symmetry of the basic set of equations. If for some reason



this is not the case, i.e., if there exists a solution which reflects some asymmetries with respect to the group  $G$ , then we say that a spontaneous symmetry breaking has occurred. Conventionally one may describe a breakdown of symmetry by introducing a noninvariant term into the Lagrangian. Another way of treating of this problem is to consider noninvariance under a group of transformations. It is known from nonrelativistic many-body theory, that solutions of the field equations exist that have less symmetry than that displayed by the Lagrangian.

The breaking of the symmetry establishes a multiplicity of “vacuums” or ground states, related by the transformations of the (broken) symmetry group.<sup>13,95,96</sup> What is important, it is that the broken symmetry state is distinguished by the appearance of a *macroscopic order parameter*. The various values of the macroscopic order parameter are in a certain correspondence with several ground states. Thus the problem arises how to establish the relevant ground state. According to Coleman arguments,<sup>25</sup> this ground state should exhibit the maximal lowering of the symmetry of all its associated macrostates.

It is worth mentioning that the idea of spontaneously broken symmetries was invented and elaborated by N. N. Bogoliubov,<sup>37,97–99</sup> P. W. Anderson,<sup>47,100,101</sup> Y. Nambu,<sup>102,103</sup> G. Jona-Lasinio and others. This idea was applied to the elementary particle physicists by Nambu in his 1960 article<sup>104</sup> (see also Ref. 105). Nambu was guided in his work by an analogy with the theory of superconductivity,<sup>97–99</sup> to which Nambu himself had made an important contribution.<sup>106</sup> According to Nambu,<sup>106,107</sup> the situation in the elementary particle physics may be understood better by making an analogy to the theory of superconductivity originated by Bogoliubov<sup>97</sup> and Bardeen, Cooper and Schrieffer.<sup>108</sup> There, gauge invariance, the energy gap, and the collective excitations were logically related to each other. This analogy was the leading idea which stimulated him greatly. A model with a broken gauge symmetry has been discussed by Nambu and Jona-Lasinio.<sup>109</sup> This model starts with a zero-mass baryon and a massless pseudoscalar meson, accompanied by a broken-gauge symmetry. The authors considered a theory with a Lagrangian possessing  $\gamma_5$  invariance and found that, although the basic Lagrangian contains no mass term, since such terms violate  $\gamma_5$  invariance, a solution exists that admits fermions of finite mass.

The appearance of spontaneously broken symmetries and its bearing on the physical mass spectrum were analyzed in variety of papers.<sup>55,110–113</sup> Kunihiro and Hatsuda<sup>114</sup> elaborated a self-consistent mean-field approach to the dynamical symmetry breaking by considering the effective potential of the Nambu and Jona-Lasinio model. In their study the dynamical symmetry breaking phenomena in the Nambu and Jona-Lasinio model were reexamined in the framework of a self-consistent mean-field (SCMF) theory. They formulated the SCMF theory in a lucid manner based on a successful decomposition on the Lagrangian into semiclassical and residual interaction parts by imposing a condition that “the dangerous term” in Bogoliubov’s sense<sup>97</sup> should vanish. It was shown that the difference of the energy density between the super and normal phases, the correct expression

of which the original authors failed to give, can be readily obtained by applying the SCMF theory. Furthermore, it was shown that the expression thus obtained is identical to that of the effective potential given by the path-integral method with an auxiliary field up to the one loop order in the loop expansion, then one finds a new and simple way to get the effective potential. Some numerical results of the effective potential and the dynamically generated mass of fermion were also obtained.

The concept of spontaneous symmetry breaking is delicate. It is worth to emphasize that it can never take place when the normalized ground state  $|\Phi_0\rangle$  of the many-particle Hamiltonian (possibly interacting) is non-degenerate, i.e., unique up to a phase factor. Indeed, the transformation law of the ground state  $|\Phi_0\rangle$  under any symmetry of the Hamiltonian must then be a multiplication by a phase factor. Correspondingly, the ground state  $|\Phi_0\rangle$  must transform according to the trivial representation of the symmetry group, i.e.,  $|\Phi_0\rangle$  transforms as a singlet. In this case there is no room for the phenomenon of spontaneous symmetry breaking by which the ground state transforms non-trivially under some symmetry group of the Hamiltonian. Now, the Perron-Frobenius theorem for finite dimensional matrices with positive entries or its extension to single-particle Hamiltonians of the form  $H = -\Delta/2m + U(r)$  guarantees that the ground state is non-degenerate for non-interacting  $N$ -body Hamiltonians defined on the Hilbert space  $\bigotimes_{\text{symm}}^N \mathcal{H}^{(1)}$ . Although there is no rigorous proof that the same theorem holds for interacting  $N$ -body Hamiltonians, it is believed that the ground state of interacting Hamiltonians defined on  $\bigotimes_{\text{symm}}^N \mathcal{H}^{(1)}$  is also unique. It is believed also that spontaneous symmetry breaking is always ruled out for interacting Hamiltonian defined on the Hilbert space  $\bigotimes_{\text{symm}}^N \mathcal{H}^{(1)}$ .

Explicit symmetry breaking indicates a situation where the dynamical equations are not manifestly invariant under the symmetry group considered. This means, in the Lagrangian (Hamiltonian) formulation, that the Lagrangian (Hamiltonian) of the system contains one or more terms explicitly breaking the symmetry. Such terms, in general, can have different origins. Sometimes symmetry-breaking terms may be introduced into the theory by hand on the basis of theoretical or experimental results, as in the case of the quantum field theory of the weak interactions. This theory was constructed in a way that manifestly violates mirror symmetry or parity. The underlying result in this case is parity non-conservation in the case of the weak interaction, as it was formulated by T. D. Lee and C. N. Yang. It may be of interest to remind in this context the general principle, formulated by C. N. Yang<sup>89</sup>: “**symmetry dictates interaction**”.

C. N. Yang<sup>89</sup> noted also that, “the lesson we have learned from it that keeps as much symmetry as possible. Symmetry is good for renormalizability ... The concept of broken symmetry does not really break the symmetry, it only breaks the symmetry phenomenologically. So the broken symmetric non-Abelian gauge field theory keeps formalistically the symmetry. That is reason why it is renormalizable. And that produced unification of electromagnetic and weak interactions”.

In fact, the symmetry-breaking terms may appear because of non-renormalizable effects. One can think of current renormalizable field theories as effective field theories, which may be a sort of low-energy approximations to a more general theory. The effects of non-renormalizable interactions are, as a rule, not big and can therefore be ignored at the low-energy regime. In this sense, the coarse-grained description thus obtained may possess more symmetries than the anticipated general theory. That is, the effective Lagrangian obeys symmetries that are not symmetries of the underlying theory. Weinberg has called them the “accidental” symmetries. They may then be violated by the non-renormalizable terms arising from higher mass scales and suppressed in the effective Lagrangian.

R. Brout and F. Englert has reviewed<sup>115</sup> the concept of spontaneous broken symmetry in the presence of global symmetries both in matter and particle physics. This concept was then taken over to confront local symmetries in relativistic field theory. Emphasis was placed on the basic concepts where, in the former case, the vacuum of spontaneous broken symmetry was degenerate whereas that of local (or gauge) symmetry was gauge invariant.

The notion of broken symmetry permits one to look more deeply at many complicated problems,<sup>32,33,116,117</sup> such as scale invariance,<sup>118</sup> stochastic interpretation of quantum mechanics,<sup>119</sup> quantum measurement problem<sup>120</sup> and many-body nuclear physics.<sup>121</sup> The problem of a great importance is to understand the domain of validity of the broken symmetry concept. Is it valid only at low energies (temperatures) or it is universally applicable.

In spite of the fact that the term *spontaneous symmetry breaking* was coined in elementary particle physics to describe the situation that the vacuum state had less symmetry than the group invariance of the equations, this notion is of use in classical mechanics where it arose in bifurcation theory.<sup>41–45</sup> The physical systems on the brink of instability are described by the new solutions which appear often possessing a lower isotropy symmetry group. The governing equations themselves continue to be invariant under the full transformation group and that is the reason why the symmetry breaking is spontaneous.

These results are of value for the nonequilibrium systems.<sup>122,123</sup> Results in nonequilibrium thermodynamics have shown that bifurcations require two conditions. First, systems have to be far from equilibrium. We have to deal with open systems exchanging energy, matter and information with the surrounding world. Secondly, we need non-linearity. This leads to a multiplicity of solutions. The choice of the branch of the solution in the non-linear problem depends on probabilistic elements. Bifurcations provide a mechanism for the appearance of novelties in the physical world. In general, however, there are successions of bifurcations, introducing a kind of memory aspect. It is now generally well-understood that all structures around us are the specific outcomes of such type of processes. The simplest example is the behavior of chemical reactions in far-from-equilibrium systems. These conditions may lead to oscillating reactions, to so-called Turing patterns, or to chaos in which initially close trajectories deviate exponentially over time. The main point is

that, for given boundary conditions (that is, for a given environment), allowing us to change of perspective is mainly due to our progress in dynamical systems and spectral theory of operators.

J. van Wezel, J. Zaanen and J. van den Brink<sup>124</sup> studied an intrinsic limit to quantum coherence due to spontaneous symmetry breaking. They investigated the influence of spontaneous symmetry breaking on the decoherence of a many-particle quantum system. This decoherence process was analyzed in an exactly solvable model system that is known to be representative of symmetry broken macroscopic systems in equilibrium. It was shown that spontaneous symmetry breaking imposes a fundamental limit to the time that a system can stay quantum coherent. This universal time scale is  $t_{\text{spont}} \sim 2\pi N\hbar/(k_B T)$ , given in terms of the number of microscopic degrees of freedom  $N$ , temperature  $T$ , and the constants of Planck ( $\hbar$ ) and Boltzmann ( $k_B$ ). According to their viewpoint, the relation between quantum physics at microscopic scales and the classical behavior of macroscopic bodies need a thorough study. This subject has revived in recent years both due to experimental progress, making it possible to study this problem empirically, and because of its possible implications for the use of quantum physics as a computational resource. This “micro-macro” connection actually has two sides. Under equilibrium conditions, it is well-understood in terms of the mechanism of spontaneous symmetry breaking. But in the dynamical realms, its precise nature is still far from clear. The question is “Can spontaneous symmetry breaking play a role in a dynamical reduction of quantum physics to classical behavior”? This is a highly nontrivial question as spontaneous symmetry breaking is intrinsically associated with the difficult problem of many-particle quantum physics. Authors analyzed a tractable model system, which is known to be representative of macroscopic systems in equilibrium, to find the surprising outcome that spontaneous symmetry breaking imposes a fundamental limit to the time that a system can stay quantum coherent.

In the next work,<sup>125</sup> J. van Wezel, J. Zaanen and J. van den Brink studied a relation between decoherence and spontaneous symmetry breaking in many-particle qubits. They used the fact that spontaneous symmetry breaking can lead to decoherence on a certain time scale and that there is a limit to quantum coherence in many-particle spin qubits due to spontaneous symmetry breaking. These results were derived for the Lieb-Mattis spin model. Authors show that the underlying mechanism of decoherence in systems with spontaneous symmetry breaking is in fact more general. J. van Wezel, J. Zaanen and J. van den Brink presented here a generic route to finding the decoherence time associated with spontaneous symmetry breaking in many-particle qubits, and subsequently applied this approach to two model systems, indicating how the continuous symmetries in these models are spontaneously broken. They discussed the relation of this symmetry breaking to the thin spectrum.

The number of works on broken symmetry within the axiomatic frame is large; this topic was reviewed by Reeh<sup>126</sup> and many others.

#### 4. Goldstone Theorem

The Goldstone theorem<sup>127</sup> is remarkable so far in that it connects the phenomenon of spontaneous breakdown of an internal symmetry with a property of the mass spectrum. In addition, the Goldstone theorem states that breaking of global continuous symmetry implies the existence of massless, spin-zero bosons. The presence of massless particles accompanying broken gauge symmetries seems to be quite general.<sup>128</sup> The *Goldstone theorem* states that, if system described by a Lagrangian which has a continuous symmetry (and only short-ranged interactions) has a broken symmetry state, then the system supports a branch of small amplitude excitations with a dispersion relation  $\varepsilon(k)$  that vanishes at  $k \rightarrow 0$ . Thus the Goldstone theorem ensures the existence of massless excitations if a continuous symmetry is spontaneously broken.

More precisely, the Goldstone theorem examines a generic continuous symmetry which is spontaneously broken, i.e., its currents are conserved, but the ground state (vacuum) is not invariant under the action of the corresponding charges. Then, necessarily, new massless (or light, if the symmetry is not exact) scalar particles appear in the spectrum of possible excitations. There is one scalar particle — called a Goldstone boson (or Nambu–Goldstone boson). In particle and condensed matter physics, Goldstone bosons are bosons that appear in models exhibiting spontaneous breakdown of continuous symmetries.<sup>129,130</sup> Such a particle can be ascribed for each generator of the symmetry that is broken, i.e., that does not preserve the ground state. The Nambu–Goldstone mode is a long-wavelength fluctuation of the corresponding order parameter.

In other words, zero-mass excitations always appear when a gauge symmetry is broken.<sup>128,131–134</sup> Some (incomplete) proofs of the initial Goldstone “conjecture” on the massless particles required by symmetry breaking were worked out by Goldstone, Salam and Weinberg.<sup>131</sup> As S. Weinberg<sup>132</sup> formulated it later, “as everyone knows now, broken global symmetries in general do not look at all like approximate ordinary symmetries, but show up instead as low energy theorems for the interactions of these massless Goldstone bosons”. These spinless bosons correspond to the spontaneously broken internal symmetry generators, and are characterized by the quantum numbers of these. They transform nonlinearly (shift) under the action of these generators, and can thus be excited out of the asymmetric vacuum by these generators. Thus, they can be thought of as the excitations of the field in the broken symmetry directions in group space and are massless if the spontaneously broken symmetry is not also broken explicitly. In the case of approximate symmetry, i.e., if it is explicitly broken as well as spontaneously broken, then the Nambu–Goldstone bosons are not massless, although they typically remain relatively light.<sup>135</sup>

In paper,<sup>136</sup> a clear statement and proof of Goldstone theorem was carried out. It was shown that any solution of a Lorenz-invariant theory (and of some other theories also) that violates an internal symmetry of the theory will contain a massless scalar excitation i.e., particle (see also Refs. 137–139).

The Goldstone theorem has applications in many-body nonrelativistic quantum theory.<sup>140–142</sup> In that case, it states that if symmetry is spontaneously broken, there are excitations (Goldstone excitations) whose frequency vanishes ( $\varepsilon(k) \rightarrow 0$ ) in the long-wavelength limit ( $k \rightarrow 0$ ). In these cases, we similarly notice that the ground state is degenerate. Examples are the isotropic ferromagnet in which the Goldstone excitations are spin waves, a Bose gas in which the breaking of the phase symmetry  $\psi \rightarrow \exp(i\alpha)\psi$  and of the Galilean invariance implies the existence of phonons as Goldstone excitations, and a crystal where breaking of translational invariance also produces phonons. Goldstone theorem was applied also to a number of nonrelativistic many-body systems<sup>141,142</sup> and the question has arisen as to whether such systems as a superconducting electron gas and an electron plasma which have an energy gap in their spectrum (analog of a nonzero mass for a particle) are not a violation of the Goldstone theorem. An inspection of the situation in which the system is coupled by long-ranged interactions, as modelled by an electromagnetic field leads to a better understanding of the limitations of Goldstone theorem. As first pointed out by Anderson,<sup>143,144</sup> the long-ranged interactions alter the excitation spectrum of the symmetry broken state by removing the Goldstone modes and generating a branch of massive excitations (see also Refs. 145 and 146).

It is worth noting that S. Coleman<sup>147</sup> proved that in two dimensions, the Goldstone phenomenon cannot occur. This is related to the fact that in four dimensions, it is possible for a scalar field to have a vacuum expectation value that would be forbidden if the vacuum were invariant under some continuous transformation group, even though this group is a symmetry group in the sense that the associated local currents are conserved. This is the Goldstone phenomenon, and Goldstone's theorem states that this phenomenon is always accompanied by the appearance of massless scalar bosons. In two dimensions, Goldstone's theorem does not end with two alternatives (either manifest symmetry or Goldstone bosons) but with only one (manifest symmetry).

There are many extensions and generalizations of the Goldstone theorem.<sup>148,149</sup> L. O'Raifeartaigh<sup>84</sup> has shown that the Goldstone theorem is actually a special case of the Noether theorem in the presence of spontaneous symmetry breakdown, and is thus immediately valid for quantized as well as classical fields. The situation when gauge fields are introduced was discussed as well. Emphasis is being placed on some points that are not often discussed in the literature, such as the compatibility of the Higgs mechanism and the Elitzur theorem<sup>83</sup> and the extent to which the vacuum configuration is determined by the choice of gauge. A. Okopinska<sup>150</sup> have shown that the Goldstone theorem is fulfilled in the  $O(N)$  symmetric scalar quantum field theory with  $\lambda\Phi^4$  interaction in the Gaussian approximation for arbitrary  $N$ . Chodos and Gallatin<sup>151</sup> pointed out that standard discussions of Goldstone's theorem were based on a symmetry of the action assuming constant fields and global transformations, i.e., transformations which are independent of space-time coordinates. By allowing for arbitrary field distributions in a general representation of the symmetry, they derived a generalization of the standard Goldstone's theorem.

When applied to gauge bosons coupled to scalars with a spontaneously broken symmetry, the generalized theorem automatically imposes the Higgs mechanism, i.e., if the expectation value of the scalar field is nonzero then the gauge bosons must be massive. The other aspect of the Higgs mechanism, the disappearance of the “would be” Goldstone boson, follows directly from the generalized symmetry condition itself. They also used the generalized Goldstone’s theorem to analyze the case of a system in which scale and conformal symmetries were both spontaneously broken. The consistency between the Goldstone theorem and the Higgs mechanism was established in a manifestly covariant way by N. Nakanishi.<sup>152</sup>

## 5. Higgs Phenomenon

The most characteristic feature of spontaneously broken gauge theories is the Higgs mechanism.<sup>153–156</sup> It is that mechanism through which the Goldstone fields disappear and gauge fields acquire masses.<sup>92,113,157,158</sup> When spontaneous symmetry breaking takes place in theories with local symmetries, then the zero-mass Goldstone bosons combine with the vector gauge bosons to form massive vector particles. Thus in a situation of spontaneous broken local symmetry, the gauge boson gets its mass from the interaction of gauge bosons with the spin-zero bosons.

The mechanism proposed by Higgs for the elimination, by symmetry breakdown, of zero-mass quanta of gauge fields have led to substantial progress in the unified theory of particles and interactions. The Higgs mechanism could explain, in principle, the fundamental particle masses in terms of the energy interaction between particles and the Higgs field.

P. W. Anderson<sup>47,100,101,143,144</sup> first pointed out that several cases in nonrelativistic condensed matter physics may be interpreted as due to *massive photons*. It was Y. Nambu<sup>103</sup> who pointed clearly that the idea of a spontaneously broken symmetry being the way in which the mass of particles could be generated. He used an analogy of a theory of elementary particles with the Bogoliubov-BCS theory of superconductivity. Nambu showed how fermion masses would be generated in a way that was analogous to the formation of the energy gap in a superconductor. In 1963, P. W. Anderson<sup>144</sup> demonstrated that the equivalent of a Goldstone boson in a superconductor could become massive due to its electromagnetic interactions. Higgs was able to show that the introduction of a subtle form of symmetry known as gauge invariance invalidated some of the assumptions made by Goldstone, Salam and Weinberg in their paper.<sup>131</sup> Higgs formulated a theory in which there was one massive spin-one particle — the sort of particle that can carry a force — and one left-over massive particle that did not have any spin. Thus he invented a new type of particle, which was later called by the Higgs boson. The so-called Higgs mechanism is the mechanism of generating vector boson masses; it was a big breakthrough in the field of particle physics.

According to F. Wilczek,<sup>71</sup> “BCS theory traces superconductivity to the existence of a special sort of long-range correlation among electrons. This effect is purely

quantum-mechanical. A classical phenomenon that is only very roughly analogous, but much simpler to visualize, is the occurrence of ferromagnetism owing to long-range correlations among electron spins (that is, their mutual alignment in a single direction). The sort of correlations responsible for superconductivity are of a much less familiar sort, as they involve not the spins of the electrons, but rather the phases of their quantum-mechanical wavefunctions . . . But as it is the leading idea guiding our construction of the Higgs system, I think it is appropriate to sketch an intermediate picture that is more accurate than the magnet analogy and suggestive of the generalization required in the Higgs system. Superconductivity occurs when the phases of the Cooper pairs all align in the same direction . . . Of course, gauge transformations that act differently at different space-time points will spoil this alignment. Thus, although the basic equations of electrodynamics are unchanged by gauge transformations, the state of a superconductor does change. To describe this situation, we say that in a superconductor gauge symmetry is spontaneously broken. The phase alignment of the Cooper pairs gives them a form of rigidity. Electromagnetic fields, which would tend to disturb this alignment, are rejected. This is the microscopic explanation of the Meissner effect, or in other words, the mass of photons in superconductors”.

The theory of the strong interaction between quarks (quantum chromodynamics, *QCD*)<sup>51</sup> is approximately invariant under what is called charge symmetry. In other words, if we swap an up quark for a down quark, then the strong interaction will look almost the same. This symmetry is related to the concept of isospin, and is not the same as charge conjugation (in which a particle is replaced by its antiparticle). Charge symmetry is broken by the competition between two different effects. The first is the small difference in mass between up and down quarks, which is about 200 times less than the mass of the proton. The second is their different electric charges. The up quark has a charge of  $+2/3$  in units of the proton charge, while the down quark has a negative charge of  $-1/3$ . If the Standard Model of particle physics<sup>51,111,112</sup> were perfectly symmetric, none of the particles in the model would have any mass. Looked at another way, the fact that most fundamental particles have non-zero masses breaks some of the symmetry in the model. Something must therefore be generating the masses of the particles and breaking the symmetry of the model. That something — which has yet to be detected in an experiment — is called the Higgs field. The origin of the quark masses is not fully understood. In the Standard Model of particle physics,<sup>51,111,112</sup> the Higgs mechanism allows the generation of such masses but it cannot predict the actual mass values. No fundamental understanding of the mass hierarchy exists. It is clear that the violation of charge symmetry can be used to treat this problem.

C. Smeenk<sup>159</sup> called the Higgs mechanism as an essential but elusive component of the Standard Model of particle physics. In his opinion, without it, Yang–Mills gauge theories would have been little more than a warm-up exercise in the attempt to quantize gravity rather than serving as the basis for the Standard Model. C. Smeenk focuses on two problems related to the Higgs mechanism, namely: (i) what



is the gauge-invariant content of the Higgs mechanism, and (ii) what does it mean to break a local gauge symmetry?

A more critical view was presented by H. Lyre.<sup>160</sup> He explored the argument structure of the concept of spontaneous symmetry breaking in the electroweak gauge theory of the Standard Model: the so-called Higgs mechanism. As commonly understood, the Higgs argument is designed to introduce the masses of the gauge bosons by a spontaneous breaking of the gauge symmetry of an additional field, the Higgs field. H. Lyre claimed that the technical derivation of the Higgs mechanism, however, consists in a mere re-shuffling of degrees of freedom by transforming the Higgs Lagrangian in a gauge-invariant manner. In his opinion, this already raises serious doubts about the adequacy of the entire manoeuvre. He insists that no straightforward ontic interpretation of the Higgs mechanism was tenable since gauge transformations possess no real instantiations. In addition, the explanatory value of the Higgs argument was critically examined in that open-to-questions paper.

## 6. Chiral Symmetry

Many symmetry principles were known, a large fraction of them were only approximate. The concept of chirality was introduced in the nineteenth century when L. Pasteur discovered one of the most interesting and enigmatic asymmetries in nature: that the chemistry of life shows a preference for molecules with a particular *handedness*. Chirality is a general concept based on the geometric characteristics of an object. A chiral object is an object which has a mirror-image non superimposable to itself. Chirality deals with molecules but also with macroscopic objects such as crystals. Many chemical and physical systems can occur in two forms distinguished solely by being mirror images of each other. This phenomenon, known as chirality, is important in biochemistry,<sup>161,162</sup> where reactions involving chiral molecules often require the participation of one specific enantiomer (mirror image) of the two possible ones. Chirality is an important concept<sup>163</sup> which has many consequences and applications in many fields of science<sup>161,164–166</sup> and especially in chemistry.<sup>167–171</sup> The problem of homochirality has attracted attention of chemists and physicists since it was found by Pasteur. The methods of solid-state physics and statistical thermodynamics were of use to study this complicated interdisciplinary problem.<sup>167–169,171</sup> A general theory of spontaneous chiral symmetry breaking in chemical systems has been formulated by D. Kondepudi.<sup>167–169,171</sup> The fundamental equations of this theory depend only on the two-fold mirror-image symmetry and not on the details of the chemical kinetics. Close to equilibrium, the system will be in a symmetric state in which the amounts of the two enantiomers of all chiral molecules are equal. When the system is driven away from equilibrium by a flow of chemicals, a point is reached at which the system becomes unstable to small fluctuation in the difference in the amount of the two enantiomers. As a consequence, a small random fluctuation in the difference in the amount of the two enantiomers spontaneously grows and the system makes a transition to an asym-

metric state. The general theory describes this phenomenon in the vicinity of the transition point.

Amino acids and DNA are the fundamental building blocks of life itself.<sup>161,162</sup> They exist in left- and right-handed forms that are mirror images of one another. Almost all the naturally occurring amino acids that make up proteins are left-handed, while DNA is almost exclusively right-handed.<sup>162</sup> Biological macromolecules, proteins and nucleic acids are composed exclusively of chirally pure monomers. The chirality consensus<sup>172</sup> appears vital for life and it has even been considered as a prerequisite of life. However the primary cause for the ubiquitous handedness has remained obscure yet. It was conjectured<sup>172</sup> that the chirality consensus is a kinetic consequence that follows from the principle of increasing entropy, i.e., the 2nd law of thermodynamics. Entropy increases when an open system evolves by decreasing gradients in free energy with more and more efficient mechanisms of energy transduction. The rate of entropy increase can be considered as the universal fitness criterion of natural selection that favors diverse functional molecules and drives the system to the chirality consensus to attain and maintain high-entropy non-equilibrium states. Thus the chiral-pure outcomes have emerged from certain scenarios and understood as consequences of kinetics.<sup>172</sup> It was pointed out that the principle of increasing entropy, equivalent to diminishing differences in energy, underlies all kinetic courses and thus could be a cause of chirality consensus. Under influx of external energy systems evolve to high entropy non-equilibrium states using mechanisms of energy transduction. The rate of entropy increase is the universal fitness criterion of natural selection among the diverse mechanisms that favors those that are most effective in leveling potential energy differences. The ubiquitous handedness enables rapid synthesis of diverse metastable mechanisms to access free energy gradients to attain and maintain high-entropy non-equilibrium states. When the external energy is cut off, the energy gradient from the system to its exterior reverses and racemization will commence toward the equilibrium. Then the mechanisms of energy transduction have become improbable and will vanish since there are no gradients to replenish them. The common consent that a racemic mixture has higher entropy than a chirally pure solution is certainly true at the stable equilibrium. Therefore, high entropy is often associated with high disorder. However, entropy is not an obscure logarithmic probability measure but probabilities describe energy densities and mutual gradients in energy.<sup>172</sup> The local order and structure that associate with the mechanisms of energy transduction are well warranted when they allow the open system as a whole to access and level free energy gradients. Order and standards are needed to attain and maintain the high-entropy non-equilibrium states. We expect that the principle of increasing entropy accounts also for the universal genetic code to allow exchange of genetic material to thrust evolution toward new more probable states. The common chirality convention is often associated with a presumed unique origin of life but it reflects more the all-encompassing unity of biota on Earth that emerged from evolution over the eons.<sup>172</sup>

Many researchers have pointed out the role of the magnetic field for the chiral asymmetry. Recently, G. Rikken and E. Raupach have demonstrated that a static magnetic field can indeed generate chiral asymmetry.<sup>173</sup> Their work reports the first unequivocal use of a static magnetic field to bias a chemical process in favour of one of two mirror-image products (left- or right-handed enantiomers). G. Rikken and E. Raupach used the fact that terrestrial life utilizes only the *L* enantiomers of amino acids, a pattern that is known as the “*homochirality of life*” and which has stimulated long-standing efforts to understand its origin. Reactions can proceed enantioselectively if chiral reactants or catalysts are involved, or if some external chiral influence is present. But because chiral reactants and catalysts themselves require an enantioselective production process, efforts to understand the homochirality of life have focused on external chiral influences. One such external influence is circularly polarized light, which can influence the chirality of photochemical reaction products. Because natural optical activity, which occurs exclusively in media lacking mirror symmetry, and magnetic optical activity, which can occur in all media and is induced by longitudinal magnetic fields, both cause polarization rotation of light, the potential for magnetically induced enantioselectivity in chemical reactions has been investigated, but no convincing demonstrations of such an effect have been found. The authors show experimentally that magnetochiral anisotropy — an effect linking chirality and magnetism — can give rise to an enantiomeric excess in a photochemical reaction driven by unpolarized light in a parallel magnetic field, which suggests that this effect may have played a role in the origin of the homochirality of life. These results clearly suggest that there could be a difference between the way the two types of amino acids break down in a strong interstellar magnetic field. A small asymmetry produced this way could be amplified through other chemical reactions to generate the large asymmetry observed in the chemistry of life on Earth.

Studies of chiral crystallization<sup>174</sup> of achiral molecules are of importance for the clarification of the nature of chiral symmetry breaking. The study of chiral crystallization of achiral molecules focuses on chirality of crystals and more specifically on chiral symmetry breaking for these crystals. Some molecules, although achiral, are able to generate chiral crystals. Chirality is then due to the crystal structure, having two enantiomorphous forms. Cubic chiral crystals are easily identifiable. Indeed, they deviate polarized light. The distribution and the ratio of the two enantiomorphous crystal forms of an achiral molecule not only in a sample but also in numerous samples prepared under specific conditions. The relevance of this type of study is, for instance, a better comprehension of homochirality. The experimental conditions act upon the breaking of chiral symmetry. Enantiomeric excess is not obviously easy to induce. Nevertheless, a constant stirring of the solution during the crystallization will generate a significant rupture of chiral symmetry in the sample and can offer an interesting and accessible case study.<sup>174</sup>

The discovery of L. Pasteur came about 100 years before physicists demonstrated that processes governed by weak-force interactions look different in a mirror-

image world. The chiral symmetry breaking has been observed in various physical problems, e.g., chiral symmetry breaking of magnetic vortices, caused by the surface roughness of thin-film magnetic structures.<sup>175</sup> Charge-symmetry breaking also manifests itself in the interactions of pions with protons and neutrons in a very interesting way that is linked to the neutron-proton (and hence, up and down quark) mass difference. Because the masses of the up and down quarks are almost zero, another approximate symmetry of QCD called *chiral* symmetry comes into play.<sup>52,176–179</sup> This symmetry relates to the spin angular momentum of fundamental particles. Quarks can either be *right-handed* or *left-handed*, depending on whether their spin is clockwise or anticlockwise with respect to the direction they are moving in. Both of these states are treated approximately the same by QCD.

Symmetry-breaking terms may appear in the theory because of quantum-mechanical effects. One reason for the presence of such terms — known as *anomalies* — is that in passing from the classical to the quantum level, because of possible operator ordering ambiguities for composite quantities such as Noether charges and currents, it may be that the classical symmetry algebra (generated through the Poisson bracket structure) is no longer realized in terms of the commutation relations of the Noether charges. Moreover, the use of a regulator (or *cut-off*) required in the renormalization procedure to achieve actual calculations may itself be a source of anomalies. It may violate a symmetry of the theory, and traces of this symmetry breaking may remain even after the regulator is removed at the end of the calculations. Historically, the first example of an anomaly arising from renormalization is the so-called chiral anomaly, that is the anomaly violating the chiral symmetry of the strong interaction.<sup>52,177,178,180</sup>

Kondepudi and Durand<sup>181</sup> applied the ideas of chiral symmetry to an astrophysical problem. They considered the so-called chiral asymmetry in spiral galaxies. Spiral galaxies are chiral entities when coupled with the direction of their recession velocity. As viewed from the Earth, the *S*-shaped and *Z*-shaped spiral galaxies are two chiral forms. The authors investigated the nature of chiral symmetry in spiral galaxies. In the Carnegie Atlas of Galaxies that lists photographs of a total of 1,168 galaxies, there are 540 galaxies, classified as normal or barred spirals, that are clearly identifiable as *S*- or *Z*-type. The recession velocities for 538 of these galaxies could be obtained from this atlas and other sources. A statistical analysis of this sample reveals no overall asymmetry but there is a significant asymmetry in certain subclasses: dominance of *S*-type galaxies in the *Sb* class of normal spiral galaxies and a dominance of *Z*-type in the *SBb* class of barred spiral galaxies. Both *S*- and *Z*-type galaxies seem to have similar velocity distribution, indicating no spatial segregation of the two chiral forms. Thus, the ideas of symmetry and chirality penetrate deeply into modern science ranging from microphysics to astrophysics.

## 7. Quantum Protectorate

It is well-known that there are many branches of physics and chemistry where phenomena occur which cannot be described in the framework of interactions amongst a few particles. As a rule, these phenomena arise essentially from the cooperative behavior of a large number of particles. Such many-body problems are of great interest not only because of the nature of the phenomena themselves, but also because of the intrinsic difficulty in solving problems which involve interactions of many particles in terms of known Anderson statement that “more is different”.<sup>94</sup> It is often difficult to formulate a fully consistent and adequate microscopic theory of complex cooperative phenomena. R. Laughlin and D. Pines invented an idea of a quantum protectorate, ‘a stable state of matter, whose generic low-energy properties are determined by a higher-organizing principle and nothing else’.<sup>60</sup> This idea brings into physics the concept that emphasizes the crucial role of low-energy and high-energy scales for treating the properties of the substance. It is known that a many-particle system (e.g., electron gas) in the low-energy limit can be characterized by a small set of *collective* (or hydrodynamic) variables and equations of motion corresponding to these variables. Going beyond the framework of the low-energy region would require the consideration of plasmon excitations, effects of electron shell reconstructing, etc. The existence of two scales, low-energy and high-energy, in the description of physical phenomena is used in physics, explicitly or implicitly.

According to R. Laughlin and D. Pines, “The emergent physical phenomena regulated by higher organizing principles have a property, namely their insensitivity to microscopics, that is directly relevant to the broad question of what is knowable in the deepest sense of the term. The low energy excitation spectrum of a conventional superconductor, for example, is completely generic and is characterized by a handful of parameters that may be determined experimentally but cannot, in general, be computed from first principles. An even more trivial example is the low-energy excitation spectrum of a conventional crystalline insulator, which consists of transverse and longitudinal sound and nothing else, regardless of details. It is rather obvious that one does not need to prove the existence of sound in a solid, for it follows from the existence of elastic moduli at long length scales, which in turn follows from the spontaneous breaking of translational and rotational symmetry characteristic of the crystalline state. Conversely, one therefore learns little about the atomic structure of a crystalline solid by measuring its acoustics. The crystalline state is the simplest known example of a quantum protectorate, a *stable state of matter whose generic low-energy properties are determined by a higher organizing principle and nothing else* ... Other important quantum protectorates include superfluidity in Bose liquids such as  $^4\text{He}$  and the newly discovered atomic condensates, superconductivity, band insulation, ferromagnetism, antiferromagnetism, and the quantum Hall states. The low-energy excited quantum states of these systems are particles in exactly the same sense that the electron in the vacuum of quantum electrodynamics is a particle ... Yet they are not elementary, and, as in the case of sound,

simply do not exist outside the context of the stable state of matter in which they live. These quantum protectorates, with their associated emergent behavior, provide us with explicit demonstrations that the underlying microscopic theory can easily have no measurable consequences whatsoever at low energies. The nature of the underlying theory is unknowable until one raises the energy scale sufficiently to escape protection". The notion of *quantum protectorate* was introduced to unify some generic features of complex physical systems on different energy scales, and is a complimentary unifying idea resembling the symmetry breaking concept in a certain sense.

The sources of quantum protection in high- $T_c$  superconductivity<sup>182</sup> and low-dimensional systems were discussed in Refs. 183–188. According to Anderson,<sup>183</sup> "the source of quantum protection is likely to be a collective state of the quantum field, in which the individual particles are sufficiently tightly coupled that elementary excitations no longer involve just a few particles, but are collective excitations of the whole system. As a result, macroscopic behavior is mostly determined by overall conservation laws".

The quasiparticle picture of high-temperature superconductors in the frame of a Fermi liquid with the fermion condensate was investigated by Amusia and Shaginyan.<sup>186</sup> In their paper, a model of a Fermi liquid with the fermion condensate was applied to the consideration of quasiparticle excitations in high-temperature superconductors, in their superconducting and normal states. Within that model, the appearance of the fermion condensate presents a quantum phase transition that separates the regions of normal and strongly correlated electron liquids. Beyond the phase transition point, the quasiparticle system is divided into two subsystems, one containing normal quasiparticles and the other — fermion condensate localized at the Fermi surface and characterized by almost dispersionless single-particle excitations. In the superconducting state, the quasiparticle dispersion in systems with fermion condensate can be presented by two straight lines, characterized by two effective masses and intersecting near the binding energy, which is of the order of the superconducting gap. This same quasiparticle picture persists in the normal state, thus manifesting itself over a wide range of temperatures as new energy scales. Arguments were presented that fermion systems with fermion condensate have features of a "quantum protectorate".

Barzykin and Pines<sup>187</sup> formulated a phenomenological model of protected behavior in the pseudogap state of underdoped cuprate superconductors. By extending their previous work on the scaling of low frequency magnetic properties of the 2–1–4 cuprates to the 1–2–3 materials, they arrived at a consistent phenomenological description of protected behavior in the pseudogap state of the magnetically underdoped cuprates. Between zero hole doping and a doping level of  $\sim 0.22$ , it reflects the presence of a mixture of an insulating spin liquid that produces the measured magnetic scaling behavior and a Fermi liquid that becomes superconducting for doping levels  $x > 0.06$ . Their analysis suggests the existence of two quantum critical points, at doping levels  $x \sim 0.05$  and  $x \sim 0.22$ , and that *d*-wave superconductivity in the

pseudogap region arises from quasiparticle-spin liquid interaction, i.e., magnetic interactions between quasiparticles in the Fermi liquid induced by their coupling to the spin liquid excitations.

Kopec<sup>188</sup> attempted to discover the origin of quantum protection in high- $T_c$  cuprates. The concept of topological excitations and the related ground state degeneracy were employed to establish an effective theory of the superconducting state evolving from the Mott insulator<sup>189</sup> for high- $T_c$  cuprates. The theory includes the effects of the relevant energy scales with the emphasis on the Coulomb interaction  $U$  governed by the electromagnetic  $U(1)$  compact group. The results were obtained for the layered  $t - t' - t_{\perp} - U - J$  system of strongly correlated electrons relevant for cuprates. Casting the Coulomb interaction in terms of composite-fermions via the gauge flux attachment facility, it was shown that instanton events in the Matsubara “imaginary time”, labeled by topological winding numbers, were essential configurations of the phase field dual to the charge. This provides a nonperturbative concept of the topological quantization and displays the significance of discrete topological sectors in the theory governed by the global characteristics of the phase field. In the paper, it was shown that for topologically ordered states these quantum numbers play the role of an order parameter in a way similar to the phenomenological order parameter for conventionally ordered states. In analogy to the usual phase transition that is characterized by a sudden change of the symmetry, the topological phase transitions are governed by a discontinuous change of the topological numbers signaled by the divergence of the zero-temperature topological susceptibility. This defines a quantum criticality ruled by topologically conserved numbers rather than the reduced principle of the symmetry breaking. The author shows that in the limit of strong correlations, topological charge is linked to the average electronic filling number and the topological susceptibility to the electronic compressibility of the system. The impact of these nontrivial  $U(1)$  instanton phase field configurations for the cuprate phase diagram was exploited. The phase diagram displays the “hidden” quantum critical point covered by the superconducting lobe in addition to a sharp crossover between a compressible normal “strange metal” state and a region characterized by a vanishing compressibility, which marks the Mott insulator. It was argued that the existence of robust quantum numbers explains the stability against small perturbation of the system and attributes to the topological “quantum protectorate” as observed in strongly correlated systems.

Some other applications of the idea of the quantum protectorate were discussed in Refs. 190–194.

## 8. Emergent Phenomena

Emergence — macro-level effect from micro-level causes — is an important and profound interdisciplinary notion of modern science.<sup>195–201</sup> Emergence is a notorious philosophical term, that was used in the domain of art. A variety of theorists have appropriated it for their purposes ever since it was applied to the problems

of life and mind.<sup>195–198,200,201</sup> It might be roughly defined as the shared meaning. Thus emergent entities (properties or substances) “*arise*” out of more fundamental entities and yet are “*novel*” or “*irreducible*” with respect to them. Each of these terms is uncertain in its own right, and their specifications yield the varied notions of emergence that have been discussed in literature.<sup>195–201</sup> There has been renewed interest in emergence within discussions of the behavior of complex systems<sup>200,201</sup> and debates over the reconcilability of mental causation, intentionality, or consciousness with physicalism. This concept is also at the heart of the numerous discussions on the interrelation of the reductionism and functionalism.<sup>195–198,201</sup>

A vast amount of current researches focuses on the search for the organizing principles responsible for emergent behavior in matter,<sup>60,61</sup> with particular attention to correlated matter, the study of materials in which unexpectedly new classes of behavior emerge in response to the strong and competing interactions among their elementary constituents. As it was formulated at Ref. 61, “we call *emergent behavior* . . . the phenomena that owe their existence to interactions between many subunits, but whose existence cannot be deduced from a detailed knowledge of those subunits alone”.

Models and simulations of collective behaviors are often based on considering them as interactive particle systems.<sup>201</sup> The focus is then on behavioral and interaction rules of particles by using approaches based on artificial agents designed to reproduce swarm-like behaviors in a virtual world by using symbolic, sub-symbolic and agent-based models. New approaches have been considered in the literature<sup>201</sup> based, for instance, on topological rather than metric distances and on fuzzy systems. Recently, a new research approach<sup>201</sup> was proposed, allowing generalization possibly suitable for a general theory of emergence. The coherence of collective behaviors, i.e., their identity detected by the observer, as given by meta-structures, properties of meta-elements, i.e., sets of values adopted by mesoscopic state variables describing collective, structural aspects of the collective phenomenon under study and related to a higher level of description (meta-description) suitable for dealing with coherence, was considered. Mesoscopic state variables were abductively identified by the observer detecting emergent properties, such as sets of suitably clustered distances, speed, directions, their ratios and ergodic properties of sets. This research approach is under implementation and validation and may be considered to model general processes of collective behavior and establish a possible initial basis for a general theory of emergence.

Emergence and complexity refer to the appearance of higher-level properties and behaviors of a system that obviously come from the collective dynamics of that system’s components.<sup>60–62,195,200,202</sup> These properties are not directly deducible from the lower-level motion of that system. Emergent properties are properties of the “whole” that are not possessed by any of the individual parts making up that whole. Such phenomena exist in various domains and can be described, using complexity concepts and thematic knowledges.<sup>195,200,201</sup> Thus this problematic is highly pluridisciplinary.<sup>203</sup>



### 8.1. *Quantum mechanics and its emergent macrophysics*

The notion of emergence in quantum physics was considered by Sewell in his book "Quantum Mechanics And Its Emergent Macrophysics".<sup>202</sup> According to his point of view, the quantum theory of macroscopic systems is a vast, ever-developing area of science that serves to relate the properties of complex physical objects to those of their constituent particles. Its essential challenge is that of finding the conceptual structures needed for the description of the various states of organization of many-particle quantum systems. In that book, Sewell proposes a new approach to the subject, based on a "*macrostatistical mechanics*", which contrasts sharply with the standard microscopic treatments of many-body problems.

According to Sewell, quantum theory began with Planck's derivation of the thermodynamics of black body radiation from the hypothesis that the action of his oscillator model of matter was quantized in integral multiples of a fundamental constant,  $\hbar$ . This result provided a microscopic theory of a macroscopic phenomenon that was incompatible with the assumption of underlying classical laws. In the century following Planck's discovery, it became abundantly clear that quantum theory is essential to natural phenomena on both the microscopic and macroscopic scales.

As a first step towards contemplating the quantum mechanical basis of macrophysics, Sewell notes the empirical fact that macroscopic systems enjoy properties that are radically different from those of their constituent particles. Thus, unlike systems of few particles, they exhibit irreversible dynamics, phase transitions and various ordered structures, including those characteristic of life. These and other macroscopic phenomena signify that complex systems, that is, ones consisting of enormous numbers of interacting particles, are qualitatively different from the sums of their constituent parts (this point of view was also stressed by Anderson<sup>94</sup>).

Sewell proceeds by presenting the operator algebraic framework for the theory. He then undertakes a macrostatistical treatment of both equilibrium and nonequilibrium thermodynamics, which yields a major new characterization of a complete set of thermodynamic variables and a nonlinear generalization of the Onsager theory. He focuses especially on ordered and chaotic structures that arise in some key areas of condensed matter physics. This includes a general derivation of superconductive electrodynamics from the assumptions of off-diagonal long-range order, gauge covariance, and thermodynamic stability, which avoids the enormous complications of the microscopic treatments. Sewell also re-analyzes a theoretical framework for phase transitions far from thermal equilibrium. It gives a coherent approach to the complicated problem of the emergence of macroscopic phenomena from quantum mechanics and clarifies the problem of how macroscopic phenomena can be interpreted from the laws and structures of microphysics.

Correspondingly, theories of such phenomena must be based not only on the quantum mechanics, but also on conceptual structures that serve to represent the characteristic features of highly complex systems.<sup>60,61,200,201,203</sup> Among the main

concepts involved here are ones representing various types of order, or organization, disorder, or chaos, and different levels of macroscopicity. Moreover, the particular concepts required to describe the ordered structures of superfluids and laser light are represented by macroscopic wave functions that are strictly quantum mechanical, although radically different from the Schrodinger wave functions of microphysics.

Thus, according to Sewell, to provide a mathematical framework for the conceptual structures required for quantum macrophysics, it is clear that one needs to go beyond the traditional form of quantum mechanics, since that does not discriminate qualitatively between microscopic and macroscopic systems. This may be seen from the fact that the traditional theory serves to represent a system of  $N$  particles within the standard Hilbert space scheme, which takes the same form regardless of whether  $N$  is “small” or “large”.

Sewell’s approach to the basic problem of how macrophysics emerges from quantum mechanics is centered on macroscopic observables. The main objective of his approach is to obtain the properties imposed on them by general demands of quantum theory and many-particle statistics. This approach resembles in a certain sense the Onsager’s irreversible thermodynamics, which is based also on macroscopic observables and certain general structures of complex systems.

The conceptual basis of quantum mechanics which go far beyond its traditional form was formulated by S. L. Adler.<sup>204</sup> According to his view, quantum mechanics is not a complete theory, but rather is an emergent phenomenon arising from the statistical mechanics of matrix models that have a global unitary invariance. The mathematical presentation of these ideas is based on dynamical variables that are matrices in complex Hilbert space, but many of the ideas carry over to a statistical dynamics of matrix models in real or quaternionic Hilbert space. Adler starts from a classical dynamics in which the dynamical variables are non-commutative matrices or operators. Despite the non-commutativity, a sensible Lagrangian and Hamiltonian dynamics was obtained by forming the Lagrangian and Hamiltonian as traces of polynomials in the dynamical variables, and repeatedly using cyclic permutation under the trace. It was assumed that the Lagrangian and Hamiltonian are constructed without use of non-dynamical matrix coefficients, so that there is an invariance under simultaneous, identical unitary transformations of all the dynamical variables, that is, there is a global unitary invariance. The author supposed that the complicated dynamical equations resulting from this system rapidly reach statistical equilibrium, and then shows that with suitable approximations, the statistical thermodynamics of the canonical ensemble for this system takes the form of quantum field theory. The requirements for the underlying trace dynamics to yield quantum theory at the level of thermodynamics are stringent, and include both the generation of a mass hierarchy and the existence of boson-fermion balance. From the equilibrium statistical mechanics of trace dynamics, the rules of quantum mechanics *emerge* as an approximate thermodynamic description of the behavior of low energy phenomena. “Low energy” here means small relative to the natural energy scale implicit in the canonical ensemble for trace dynamics, which author

identifies with the Planck scale, and by “equilibrium” he means local equilibrium, permitting spatial variations associated with dynamics on the low energy scale. Brownian motion corrections to the thermodynamics of trace dynamics then lead to fluctuation corrections to quantum mechanics which take the form of stochastic modifications of the Schrodinger equation, that can account in a mathematically precise way for state vector reduction with Born rule probabilities.<sup>204</sup>

Adler emphasizes<sup>204</sup> that he has not identified a candidate for the specific matrix model that realizes his assumptions; there may be only one, which could then provide the underlying unified theory of physical phenomena that is the goal of current researches in high-energy physics and cosmology.

He admits the possibility also that the underlying dynamics may be discrete, and this could naturally be implemented within his framework of basing an underlying dynamics on trace class matrices. The ideas of the Adler's book suggest that one should seek a common origin for both gravitation and quantum field theory at the deeper level of physical phenomena from which quantum field theory emerges<sup>204</sup> (see also Ref. 205).

Recently, in Ref. 206, the causality as an emergent macroscopic phenomenon was analyzed within the Lee-Wick  $O(N)$  model. In quantum mechanics, the deterministic property of classical physics is an emergent phenomenon appropriate only on macroscopic scales. Lee and Wick introduced Lorenz invariant quantum theories where causality is an emergent phenomenon appropriate for macroscopic time scales. In Ref. 206, authors analyzed a Lee-Wick version of the  $O(N)$  model. It was argued that in the large- $N$  limit this theory has a unitary and Lorenz invariant  $S$  matrix and is therefore free of paradoxes of scattering experiments.

## 8.2. Emergent phenomena in quantum condensed matter physics

Statistical physics and condensed matter physics supply us with many examples of emergent phenomena. For example, taking a macroscopic approach to the problem, and identifying the right degrees of freedom of a many-particle system, the equations of motion of interacting particles forming a fluid can be described by the Navier-Stokes equations for fluid dynamics from which complex new behaviors arise such as turbulence. This is the clear example of an emergent phenomenon in classical physics.

Including quantum mechanics into the consideration leads to an even more complicated situation. In 1972, P. W. Anderson published his essay “More is Different” which describes how new concepts, not applicable in ordinary classical or quantum mechanics, can arise from the consideration of aggregates of large numbers of particles<sup>94</sup> (see also Ref. 117). Quantum mechanics is a basis of macrophysics. However, macroscopic systems have the properties that are radically different from those of their constituent particles. Thus, unlike systems of few particles, they exhibit irreversible dynamics, phase transitions and various ordered structures, including those characteristic of life. These and other macroscopic phenomena signify that

complex systems, that is, ones consisting of huge numbers of interacting particles, are qualitatively different from the sums of their constituent parts.<sup>94</sup>

Many-particle systems where the interaction is strong have often complicated behavior, and require nonperturbative approaches to treat their properties. Such situations often arise in condensed matter systems. Electrical, magnetic and mechanical properties of materials are *emergent collective behaviors* of the underlying quantum mechanics of their electrons and constituent atoms. A principal aim of solid state physics and materials science is to elucidate this emergence. A full achievement of this goal would imply the ability to engineer a material that is optimum for any particular application. The current understanding of electrons in solids uses simplified but workable picture known as the Fermi liquid theory. This theory explains why electrons in solids can often be described in a simplified manner which appears to ignore the large repulsive forces that electrons are known to exert on one another. There is a growing appreciation that this theory probably fails for entire classes of possibly useful materials and there is the suspicion that the failure has to do with unresolved competition between different possible emergent behaviors.

Strongly correlated electron materials manifest emergent phenomena by the remarkable range of quantum ground states that they display, e.g., insulating, metallic, magnetic, superconducting, with apparently trivial, or modest changes in chemical composition, temperature or pressure. Of great recent interest are the behaviors of a system poised between two stable zero temperature ground states, i.e., at a quantum critical point. These behaviors intrinsically support non-Fermi liquid (NFL) phenomena, including the electron fractionalization that is characteristic of thwarted ordering in a one-dimensional interacting electron gas.

In spite of the difficulties, a substantial progress has been made in understanding strongly interacting quantum systems,<sup>47,94,207,208</sup> and this is the main scope of the quantum condensed matter physics. It was speculated that a strongly interacting system can be roughly understood in terms of weakly interacting quasiparticle excitations. In some of the cases, the quasiparticles bear almost no resemblance to the underlying degrees of freedom of the system — they have *emerged* as a complex collective effect. In the last three decades, there has been the emergence of the new profound concepts associated with fractionalization, topological order, emergent gauge bosons and fermions, and string condensation.<sup>208</sup> These new physical concepts are so fundamental that they may even influence our understanding of the origin of light and electrons in the universe.<sup>62</sup> Other systems of interest are dissipative quantum systems, Bose–Einstein condensation, symmetry breaking and gapless excitations, phase transitions, Fermi liquids, spin density wave states, Fermi and fractional statistics, quantum Hall effects, topological/quantum order, spin liquid and string condensation.<sup>208</sup> The typical example of emergent phenomena is in fractional quantum Hall systems<sup>209</sup> — two dimensional systems of electrons at low temperature and in high magnetic fields. In this case, the underlying degrees of freedom are the electron, but the emergent quasiparticles have charge which

is only a fraction of that of the electron. The fractionalization of the elementary electron is one of the remarkable discoveries of quantum physics, and is purely a collective emergent effect. It is quite interesting that the quantum properties of these fractionalized quasiparticles are unlike any ever found elsewhere in nature.<sup>208</sup> In non-Abelian topological phases of matter, the existence of a degenerate ground state subspace suggests the possibility of using this space for storing and processing quantum information.<sup>210</sup> In topological quantum computation,<sup>210</sup> quantum information is stored in exotic states of matter which are intrinsically protected from decoherence, and quantum operations are carried out by dragging particle-like excitations (quasiparticles) around one another in two space dimensions. The resulting quasiparticle trajectories define world-lines in three dimensional space-time, and the corresponding quantum operations depend only on the topology of the braids formed by these world-lines. Authors<sup>210</sup> described recent work showing how to find braids which can be used to perform arbitrary quantum computations using a specific kind of quasiparticle (those described by the so-called Fibonacci anyon model) which are thought to exist in the experimentally observed  $\nu = 12/5$  fractional quantum Hall state.

In Ref. 62, Levine and Wen proposed to consider photons and electrons as emergent phenomena. Their arguments are based on recent advances in condensed-matter theory<sup>208</sup> which have revealed that new and exotic phases of matter can exist in spin models (or more precisely, local bosonic models) via a simple physical mechanism, known as “*string-net condensation*”. These new phases of matter have the unusual property that their collective excitations are gauge bosons and fermions. In some cases, the collective excitations can behave just like the photons, electrons, gluons, and quarks in the relevant vacuum. This suggests that photons, electrons, and other elementary particles may have a unified origin-string-net condensation in that vacuum. In addition, the string-net picture indicates how to make artificial photons, artificial electrons, and artificial quarks and gluons in condensed-matter systems.

In the paper,<sup>211</sup> Hastings and Wen analyzed the quasiadiabatic continuation of quantum states. They considered the stability of topological ground-state degeneracy and emergent gauge invariance for quantum many-body systems. The continuation is valid when the Hamiltonian has a gap, or else has a sufficiently small low-energy density of states, and thus is away from a quantum phase transition. This continuation takes local operators into local operators, while approximately preserving the ground-state expectation values. They applied this continuation to the problem of gauge theories coupled to matter, and propose the distinction of perimeter law versus “zero law” to identify confinement. The authors also applied the continuation to local bosonic models with emergent gauge theories. It was shown that local gauge invariance is topological and cannot be broken by any local perturbations in the bosonic models in either continuous or discrete gauge groups. Additionally, they show that the ground-state degeneracy in emergent discrete gauge theories is a robust property of the bosonic model, and the arguments were given

that the robustness of local gauge invariance in the continuous case protects the gapless gauge boson.

Pines and co-workers<sup>212</sup> carried out a theory of scaling in the emergent behavior of heavy-electron materials. It was shown that the NMR Knight shift anomaly exhibited by a large number of heavy electron materials can be understood in terms of the different hyperfine couplings of probe nuclei to localized spins and to conduction electrons. The onset of the anomaly is at a temperature  $T^*$ , below which an itinerant component of the magnetic susceptibility develops. This second component characterizes the polarization of the conduction electrons by the local moments and is a signature of the emerging heavy electron state. The heavy electron component grows as  $\log T$  below  $T^*$ , and scales universally for all measured Ce, Yb and U based materials. Their results suggest that  $T^*$  is not related to the single ion Kondo temperature,  $T_K$  (see Ref. 213), but rather represents a correlated Kondo temperature that provides a measure of the strength of the intersite coupling between the local moments.

The complementary questions concerning the emergent symmetry and dimensional reduction at a quantum critical point were investigated in Refs. 214 and 215. Interesting discussion of the emergent physics which was only partially reviewed here may be found in the paper of Volovik.<sup>199</sup>

## 9. Magnetic Degrees of Freedom and Models of Magnetism

The development of the quantum theory of magnetism was concentrated on the right definition of the fundamental “magnetic” degrees of freedom and their correct model description for complex magnetic systems.<sup>216–218</sup> We shall first describe the phenomenology of the magnetic materials to look at the physics involved. The problem of identification of the fundamental “magnetic” degrees of freedom in complex materials is rather nontrivial. Let us discuss briefly, to give a flavor only, the very intriguing problem of the electron dual behavior. The existence and properties of localized and itinerant magnetism in insulators, metals, oxides and alloys and their interplay in complex materials is an interesting and not yet fully understood problem of quantum theory of magnetism.<sup>207,217–219</sup> The central problem of recent efforts is to investigate the interplay and competition of the insulating, metallic, superconducting, and heavy fermion behavior versus the magnetic behavior, especially in the vicinity of a transition to a magnetically ordered state. The behavior and the true nature of the electronic and spin states and their quasiparticle dynamics are of central importance to the understanding of the physics of strongly correlated systems such as magnetism and metal-insulator transition in metals and oxides, heavy fermion states, superconductivity, and their competition with magnetism. The strongly correlated electron systems are systems in which electron correlations dominate. An important problem in understanding the physical behavior of these systems was the connection between relevant underlying chemical, crystal, and electronic structure, and the magnetic and transport properties which continue to be

the subject of intensive debates. Strongly correlated  $d$  and  $f$  electron systems are of special interest.<sup>207,218,219</sup> In these materials, electron correlation effects are essential and, moreover, their spectra are complex, i.e., have many branches. Importance of the studies on strongly correlated electron systems are concerned with a fundamental problem of electronic solid state theory, namely, with a tendency of  $3(4)d$  electrons in transition metals and compounds and  $4(5)f$  electrons in rare-earth metals and compounds and alloys to exhibit both localized and delocalized behavior. Many electronic and magnetic features of these substances relate intimately to this dual behavior of the relevant electronic states. For example, there are some alloy systems in which radical changes in physical properties occur with relatively modest changes in chemical composition or structural perfection of the crystal lattice. Due to competing interactions of comparable strength, more complex ground states than usually supposed may be realized. The strong correlation effects among electrons, which lead to the formation of the heavy fermion state take part to some extent in formation of a magnetically ordered phase, and thus imply that the very delicate competition and interplay of interactions exist in these substances. For most of the heavy fermion superconductors, cooperative magnetism, usually some kind of antiferromagnetic ordering was observed in the "vicinity" of superconductivity. In the case of U-based compounds, the two phenomena, antiferromagnetism and superconductivity coexist on a microscopic scale, while they seem to compete with each other in the Ce-based systems. For a Kondo lattice system,<sup>220–222</sup> the formation of a Neel state via the RKKY intersite interaction compete with the formation of a local Kondo singlet.<sup>213</sup> Recent data for many heavy fermion Ce- or U-based compounds and alloys display a pronounced non-Fermi-liquid behavior. A number of theoretical scenarios have been proposed and they can be broadly classified into two categories which deal with the localized and extended states of  $f$ -electrons. Of special interest is the unsolved controversial problem of the reduced magnetic moment in Ce- and U-based alloys and the description of the heavy fermion state in the presence of the coexisting magnetic state. In other words, the main interest is in the understanding of the competition of intra-site (Kondo screening) and inter-site (RKKY exchange) interactions. Depending on the relative magnitudes of the Kondo and RKKY scales, materials with different characteristics are found which are classified as non-magnetic and magnetic concentrated Kondo systems. These features reflect the very delicate interplay and competition of interactions and changes in a chemical composition. As a rule, very little intuitive insight could be gained from this very complicated behavior.

Magnetism in materials such as iron and nickel results from the cooperative alignment of the microscopic magnetic moments of electrons in the material. The interactions between the microscopic magnets are described mathematically by the form of the Hamiltonian of the system. The Hamiltonian depends on some parameters, or coupling constants, which measure the strength of different kinds of interactions. The magnetization, which is measured experimentally, is related to the average or mean alignment of the microscopic magnets. It is clear that some

of the parameters describing the transition to the magnetically ordered state do depend on the detailed nature of the forces between the microscopic magnetic moments. The strength of the interaction will be reflected in the critical temperature which is high if the aligning forces are strong and low if they are weak. In quantum theory of magnetism, the method of model Hamiltonians has proved to be very effective.<sup>216–218,223–225</sup> Without exaggeration, one can say that the great advances in the physics of magnetic phenomena are to a considerable extent due to the use of very simplified and schematic model representations for the theoretical interpretation.<sup>216–218,223–225</sup>

### 9.1. Ising model

One can regard the Ising model<sup>216,223</sup> as the first model of the quantum theory of magnetism. In this model, formulated by W. Lenz in 1920 and studied by E. Ising, it was assumed that the spins are arranged at the sites of a regular one-dimensional lattice. Each spin can obtain the values  $\pm\hbar/2$ :

$$H = - \sum_{ij} J(i-j) S_i S_j - g\mu_B H \sum_i S_i. \quad (9.1)$$

This Hamiltonian was one of the first attempts to describe the magnetism as a cooperative effect. It is interesting that the one-dimensional Ising model

$$H = -J \sum_{i=1}^N S_i S_{i+1} \quad (9.2)$$

was solved by Ising in 1925, while the exact solution of the Ising model on a two-dimensional square lattice was obtained by L. Onsager only in 1944.

Ising model with no external magnetic field have a global discrete symmetry, namely the symmetry under reversal of spins  $S_i \rightarrow -S_i$ . We recall that the symmetry is spontaneously broken if there is a quantity (the order parameter) that is not invariant under the symmetry operation and has a nonzero expectation value. For Ising model, the order parameter is equal to  $M = \sum_{i=1}^N S_i$ . It is not invariant under the symmetry operation. In principle, there should not be any spontaneous symmetry breaking as it is clear from the consideration of the thermodynamic average  $m = \langle M \rangle = \text{Tr}(M\rho(H)) = 0$ . We have

$$m = \left\langle N^{-1} \sum_{i=1}^N S_i \right\rangle = \frac{1}{N \cdot Z_N} \sum_i \sum_{S_i=\pm 1} S_i \exp(-\beta H(S_i)) = 0 \quad (9.3)$$

Thus to achieve the spontaneous symmetry breaking, one should take the thermodynamic limit ( $N \rightarrow \infty$ ). But this is not enough. In addition, one needs the symmetry breaking field  $h$  which leads to extra term in the Hamiltonian  $\mathcal{H} = H - h \cdot M$ . It is important to note that

$$\lim_{h \rightarrow 0} \lim_{N \rightarrow \infty} \langle M \rangle_{h,N} = m \neq 0. \quad (9.4)$$



In this equation, limits cannot be interchanged.

Let us remark that for Ising model energy cost to rotate one spin is equal to  $E_g \propto J$ . Thus every excitation costs finite energy. As a consequence, long-wavelength spin-waves cannot happen with discrete broken symmetry.

In one-dimensional case ( $D = 1$ ) the average value  $\langle M \rangle = 0$ , i.e., there is no spontaneously symmetry breaking for all  $T > 0$ . In two-dimensional case ( $D = 2$ ) the average value  $\langle M \rangle \neq 0$ , i.e., there is spontaneously symmetry breaking and the phase transition. In other words, for two-dimensional case for  $T$  small enough, the system will prefer the ordered phase, whereas for one-dimensional case no matter how small  $T$  is, the system will prefer the disordered phase (for the number of flipping neighboring spins large enough).

### 9.2. Heisenberg model

The Heisenberg model<sup>216,223</sup> is based on the assumption that the wave functions of magnetically active electrons in crystals differ little from the atomic orbitals. The physical picture can be represented by a model in which the localized magnetic moments originating from ions with incomplete shells interact through a short-range interaction. Individual spin moments form a regular lattice. The model of a system of spins on a lattice is termed the Heisenberg ferromagnet<sup>216</sup> and establishes the origin of the coupling constant as the exchange energy. The Heisenberg ferromagnet in a magnetic field  $H$  is described by the Hamiltonian

$$H = - \sum_{ij} J(i-j) \vec{S}_i \vec{S}_j - g\mu_B H \sum_i S_i^z \tag{9.5}$$

The coupling coefficient  $J(i-j)$  is the measure of the exchange interaction between spins at the lattice sites  $i$  and  $j$  and is usually defined to have the property  $J(i-j=0) = 0$ . This constraint means that only the inter-exchange interactions are taken into account. The coupling, in principle, can be of a more general type (non-Heisenberg terms). For crystal lattices in which every ion is at the centre of symmetry, the exchange parameter has the property  $J(i-j) = J(j-i)$ .

We can then rewrite the Hamiltonian (9.5) as

$$H = - \sum_{ij} J(i-j) (S_i^z S_j^z + S_i^+ S_j^-) \tag{9.6}$$

Here  $S^\pm = S^x \pm iS^y$  are the raising and lowering spin angular momentum operators. The complete set of spin commutation relations is

$$\begin{aligned} [S_i^+, S_j^-]_- &= 2S_i^z \delta_{ij}; & [S_i^+, S_i^-]_+ &= 2S(S+1) - 2(S_i^z)^2; \\ [S_i^\mp, S_j^z]_- &= \pm S_i^\mp \delta_{ij}; & S_i^z &= S(S+1) - (S_i^z)^2 - S_i^- S_i^+; \\ (S_i^+)^{2S+1} &= 0, & (S_i^-)^{2S+1} &= 0. \end{aligned}$$

We omit the term of interaction of the spin with an external magnetic field for the brevity of notation. The statistical mechanical problem involving this Hamiltonian was not exactly solved, but many approximate solutions were obtained.<sup>217</sup>

To proceed further, it is important to note that for the isotropic Heisenberg model, the total  $z$ -component of spin  $S_{\text{tot}}^z = \sum_i S_i^z$  is a constant of motion, i.e.

$$[H, S_{\text{tot}}^z] = 0. \tag{9.7}$$

There are cases when the total spin is not a constant of motion, as, for instance, for the Heisenberg model with the dipole terms added.

Let us define the eigenstate  $|\psi_0\rangle$  so that  $S_i^+|\psi_0\rangle = 0$  for all lattice sites  $R_i$ . It is clear that  $|\psi_0\rangle$  is a state in which all the spins are fully aligned and for which  $S_i^z|\psi_0\rangle = S|\psi_0\rangle$ . We also have

$$J_{\vec{k}} = \sum_i e^{(i\vec{k}\vec{R}_i)} J(i) = J_{-\vec{k}},$$

where the reciprocal vectors  $\vec{k}$  are defined by cyclic boundary conditions. Then we obtain

$$H|\psi_0\rangle = - \sum_{ij} J(i-j) S^2 = -NS^2 J_0.$$

Here  $N$  is the total number of ions in the crystal. So, for the isotropic Heisenberg ferromagnet, the ground state  $|\psi_0\rangle$  has an energy  $-NS^2 J_0$ . The state  $|\psi_0\rangle$  corresponds to a total spin  $NS$ .

Let us consider now the first excited state. This state can be constructed by creating one unit of spin deviation in the system. As a result, the total spin is  $NS - 1$ . The state

$$|\psi_k\rangle = \frac{1}{\sqrt{(2SN)}} \sum_j e^{(i\vec{k}\vec{R}_j)} S_j^- |\psi_0\rangle$$

is an eigenstate of  $H$  which corresponds to a single magnon of the energy

$$E(q) = 2S(J_0 - J_q). \tag{9.8}$$

Note that the role of translational symmetry, i.e., the regular lattice of spins, is essential, since the state  $|\psi_k\rangle$  is constructed from the fully aligned state by decreasing the spin at each site and summing over all spins with the phase factor  $e^{i\vec{k}\vec{R}_j}$  (we consider the 3-dimensional case only). It is easy to verify that

$$\langle \psi_k | S_{\text{tot}}^z | \psi_k \rangle = NS - 1.$$

Thus the Heisenberg model possesses the continuous symmetry under rotation of spins  $\vec{S}_i \rightarrow \mathcal{R}\vec{S}_i$ . Order parameter  $M^z \sim \sum_i S_i^z$  is not invariant under this transformation. Spontaneously symmetry breaking of continuous symmetry is manifested by new excitations — Goldstone modes which cost little energy. Let us rewrite the Heisenberg Hamiltonian in the following form ( $|S_i| = 1$ ):

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \vec{S}_j = -J \sum_{ij} \cos(\theta_{ij}) \tag{9.9}$$

In the ground state, all spins are aligned in one direction (ferromagnetic state). The energy cost to rotate one spin is equal to  $E_g \propto J(1 - \cos \theta)$ , where  $\theta$  is infinitesimal small angle. Thus the energy cost to rotate all spins is very small due to continuous symmetry of the Hamiltonian. As a result, the long-wavelength spin-waves exist in the Heisenberg model.

The above consideration was possible because we knew the exact ground state of the Hamiltonian. There are many models where this is not the case. For example, we do not know the exact ground state of a Heisenberg ferromagnet with dipolar forces and the ground state of the Heisenberg antiferromagnet.

The isotropic Heisenberg ferromagnet (9.5) is often used as an example of a system with spontaneously broken symmetry. This means that the Hamiltonian symmetry, the invariance with respect to rotations, is no longer the symmetry of the equilibrium state. Indeed, the ferromagnetic states of the model are characterized by an axis of the preferred spin alignment, and hence, they have a lower symmetry than the Hamiltonian itself. The essential role of the physics of magnetism in the development of symmetry ideas was noted in the paper by Y. Nambu,<sup>102</sup> devoted to the development of the elementary particle physics and the origin of the concept of spontaneous symmetry breakdown. Nambu points out that back at the end of the 19th century, P. Curie used symmetry principles in the physics of condensed matter. Nambu also notes: "More relevant examples for us, however, came after Curie. The ferromagnetism is the prototype of today's spontaneous symmetry breaking, as was explained by the works of Weiss, Heisenberg, and others. Ferromagnetism has since served us as a standard mathematical model of spontaneous symmetry breaking".

This statement by Nambu should be understood in light of the clarification made by Anderson<sup>226</sup> (see also Ref. 117). He claimed that there is "the false analogy between broken symmetry and ferromagnetism". According to Anderson,<sup>226</sup> "in ferromagnetism, specifically, the ground state is an eigenstate of the relevant continuous symmetry (that of spin rotation), and as a result, the symmetry is unbroken and the low-energy excitations have no new properties. Broken symmetry proper occurs when the ground state is not an eigenstate of the original group, as in antiferromagnetism or superconductivity; only then does one have the concepts of quasidegeneracy and of Goldstone bosons and the 'Higgs' phenomenon".

### 9.3. *Itinerant electron model*

E. Stoner<sup>227</sup> has proposed an alternative, phenomenological band model of magnetism of the transition metals in which the bands for electrons of different spins are shifted in energy in a way that is favorable to ferromagnetism.<sup>216,228</sup> E. P. Wohlfarth<sup>229</sup> developed further the Stoner ideas by considering in greater detail the quantum-mechanical and statistical-mechanical foundations of the collective electron theory and by analyzing a wider range of relevant experimental results. Wohlfarth considered the difficulties of a rigorous quantum mechanical derivation of the internal energy of a ferromagnetic metal at absolute zero. In order to deter-

mine the form of the expressions, he carried out a calculation based on the tight binding approximation for a crystal containing  $N$  singly charged ions, which are fairly widely separated, and  $N$  electrons. The forms of the Coulomb and exchange contributions to the energy were discussed in the two instances of maximum and minimum multiplicity. The need for correlation corrections was stressed, and the effects of these corrections were discussed with special reference to the state of affairs at infinite ionic separation. The fundamental difficulties involved in calculating the energy as a function of magnetization were considered as well; it was shown that they are probably less serious for tightly bound than for free electrons, so that the approximation of neglecting them in the first instance is not too unreasonable. The dependence of the exchange energy on the relative magnetization  $m$  was corrected.

The Stoner model promoted the subsequent development of the itinerant model of magnetism. It was established that the band shift effect is a consequence of strong intra-atomic correlations. The itinerant-electron picture is the alternative conceptual picture for magnetism.<sup>216</sup> It must be noted that the problem of band antiferromagnetism is a much more complicated subject.<sup>230</sup> The antiferromagnetic state is characterized by a spatially changing component of magnetization which varies in such a way that the net magnetization of the system is zero. The concept of antiferromagnetism of localized spins, which is based on the Heisenberg model and two-sublattice Neel ground state, is relatively well-founded contrary to the antiferromagnetism of delocalized or itinerant electrons. In relation to the duality of localized and itinerant electronic states, G. Wannier<sup>231</sup> showed the importance of the description of the electronic states which reconcile the band and local (cell) concept as a matter of principle. Wannier functions  $\phi(\vec{r} - \vec{R}_n)$  form a complete set of mutually orthogonal functions localized around each lattice site  $\vec{R}_n$  within any band or group of bands. They permit one to formulate an effective Hamiltonian for electrons in periodic potentials and span the space of a singly energy band. However, the real computation of Wannier functions in terms of sums over Bloch states is a difficult task. A method for determining the optimally localized set of generalized Wannier functions associated with a set of Bloch bands in a crystalline solid was discussed in Ref. 232. Thus, in condensed matter theory, the Wannier functions play an important role in the theoretical description of transition metals, their compounds and disordered alloys, impurities and imperfections, surfaces, etc. P. W. Anderson<sup>233</sup> proposed a model of transition metal impurity in the band of a host metal. All these and many other works have led to the formulation of the narrow-band model of magnetism.

#### 9.4. *Hubbard model*

There are big difficulties in the description of the complicated problem of magnetism in a metal with the  $d$  band electrons which are really neither “local” nor “itinerant” in a full sense. The Wannier functions basis set is the background of the widely used

Hubbard model. The Hubbard model<sup>234</sup> is in a certain sense an intermediate model (the narrow-band model) and takes into account the specific features of transition metals and their compounds by assuming that the  $d$  electrons form a band, but are subject to a strong Coulomb repulsion at one lattice site. The Hubbard Hamiltonian is of the form

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U/2 \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}. \quad (9.10)$$

It includes the intra-atomic Coulomb repulsion  $U$  and the one-electron hopping energy  $t_{ij}$ . The electron correlation forces electrons to localize in the atomic orbitals which are modelled here by a complete and orthogonal set of the Wannier wave functions  $[\phi(\vec{r} - \vec{R}_j)]$ . On the other hand, the kinetic energy is reduced when electrons are delocalized. The band energy of Bloch electrons  $\epsilon_{\vec{k}}$  is defined as follows:

$$t_{ij} = N^{-1} \sum_{\vec{k}} \epsilon_{\vec{k}} \exp[i\vec{k}(\vec{R}_i - \vec{R}_j)], \quad (9.11)$$

where  $N$  is the number of lattice sites. This conceptually simple model is mathematically very complicated.<sup>207,218</sup> The Pauli exclusion principle<sup>235</sup> which does not allow two electrons of common spin to be at the same site, plays a crucial role. It can be shown, that under transformation  $\mathcal{R}H\mathcal{R}^\dagger$ , where  $\mathcal{R}$  is the spin rotation operator

$$\mathcal{R} = \bigotimes_j \exp\left(\frac{1}{2}i\phi\vec{\sigma}_j\vec{n}\right), \quad (9.12)$$

the Hubbard Hamiltonian is invariant under spin rotation, i.e.,  $\mathcal{R}H\mathcal{R}^\dagger = H$ . Here  $\phi$  is the angle of rotation around the unitary axis  $\vec{n}$  and  $\vec{\sigma}$  is the Pauli spin vector; symbol  $\bigotimes_j$  indicates a tensor product over all site subspaces. The summation over  $j$  extends to all sites.

The equivalent expression for the Hubbard model that manifests the property of rotational invariance explicitly can be obtained with the aid of the transformation

$$\vec{S}_i = \frac{1}{2} \sum_{\sigma\sigma'} a_{i\sigma}^\dagger \vec{\sigma}_{\sigma\sigma'} a_{j\sigma'}. \quad (9.13)$$

Then the second term in (9.10) takes the following form

$$n_{i\uparrow}n_{i\downarrow} = \frac{n_i}{2} - \frac{2}{3}\vec{S}_i^2.$$

As a result we get

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i \left( \frac{n_i^2}{4} - \frac{1}{3}\vec{S}_i^2 \right). \quad (9.14)$$

The total  $z$ -component  $S_{\text{tot}}^z$  commutes with Hubbard Hamiltonian and the relation  $[H, S_{\text{tot}}^z] = 0$  is valid.

### 9.5. Multi-band models. Model with $s$ - $d$ hybridization

The Hubbard model is the single-band model. It is necessary, in principle, to take into account the multi-band structure, orbital degeneracy, interatomic effects and electron-phonon interaction. The band structure calculations and the experimental studies showed that for noble, transition and rare-earth metals, the multi-band effects are essential. An important generalization of the single-band Hubbard model is the so-called model with  $s$ - $d$  hybridization.<sup>236,237</sup> For transition  $d$  metals, investigation of the energy band structure reveals that  $s$ - $d$  hybridization processes play an important part. Thus, among the other generalizations of the Hubbard model that correspond more closely to the real situation in transition metals, the model with  $s$ - $d$  hybridization serves as an important tool for analyzing the multi-band effects. The system is described by a narrow  $d$ -like band, a broad  $s$ -like band and a  $s$ - $d$  mixing term coupling the two former terms. The model Hamiltonian reads

$$H = H_d + H_s + H_{s-d}. \quad (9.15)$$

The Hamiltonian  $H_d$  of tight-binding electrons is the Hubbard model (9.10).

$$H_s = \sum_{k\sigma} \epsilon_k^s c_{k\sigma}^\dagger c_{k\sigma} \quad (9.16)$$

is the Hamiltonian of a broad  $s$ -like band of electrons.

$$H_{s-d} = \sum_{k\sigma} V_k (c_{k\sigma}^\dagger a_{k\sigma} + a_{k\sigma}^\dagger c_{k\sigma}) \quad (9.17)$$

is the interaction term which represents a mixture of the  $d$ -band and  $s$ -band electrons. The model Hamiltonian (9.15) can be interpreted also in terms of a series of Anderson impurities<sup>233</sup> placed regularly in each site (the so-called periodic Anderson model). The model (9.15) is rotationally invariant also.

### 9.6. Spin-Fermion model

Many magnetic and electronic properties of rare-earth metals and compounds (e.g., magnetic semiconductors) can be interpreted in terms of a combined spin-fermion model<sup>220-222</sup> that includes the interacting localized spin and itinerant charge subsystems. The concept of the  $s(d)$ - $f$  model plays an important role in the quantum theory of magnetism, especially the generalized  $d$ - $f$  model, which describes the localized  $4f(5f)$ -spins interacting with  $d$ -like tight-binding itinerant electrons and takes into consideration the electron-electron interaction. The total Hamiltonian of the model is given by

$$H = H_d + H_{d-f}. \quad (9.18)$$

The Hamiltonian  $H_d$  of tight-binding electrons is the Hubbard model (9.10). The term  $H_{d-f}$  describes the interaction of the total  $4f(5f)$ -spins with the spin density of the itinerant electrons

$$H_{d-f} = \sum_i J \vec{\sigma}_i \vec{S}_i = -JN^{-1/2} \sum_{kq} \sum_{\sigma} [S_{-q}^{-\sigma} a_{k\sigma}^\dagger a_{k+q-\sigma} + z_{\sigma} S_{-q}^z a_{k\sigma}^\dagger a_{k+q\sigma}], \quad (9.19)$$

where sign factor  $z_\sigma$  is given by

$$z_\sigma = (+, -); \quad -\sigma = (\uparrow, \downarrow); \quad S_{-q}^{-\sigma} = \begin{cases} S_{-q}^-, & -\sigma = +, \\ S_{-q}^+, & -\sigma = -. \end{cases} \quad (9.20)$$

In general the indirect exchange integral  $J$  strongly depends on the wave vectors  $J(\vec{k}; \vec{k} + \vec{q})$  having its maximum value at  $k = q = 0$ . We omit this dependence for the sake of brevity of notation. To describe the magnetic semiconductors, the Heisenberg interaction term (9.5) should be added<sup>220–222</sup> (the resulting model is called the modified Zener model).

These model Hamiltonians (9.5), (9.10), (9.15), (9.18) (and their simple modifications and combinations) are the most commonly used models in quantum theory of magnetism. In our previous paper,<sup>238</sup> where the detailed analysis of the neutron scattering experiments on magnetic transition metals and their alloys and compounds was made, it was concluded that at the level of low-energy hydrodynamic excitations, one cannot distinguish between the models. The reason for that is the spin-rotation symmetry. In terms of Ref. 60, the spin waves (collective waves of the order parameter) are in a quantum protectorate<sup>219</sup> precisely in this sense.

### 9.7. Symmetry and physics of magnetism

In many-body interacting systems, symmetry is important in classifying different phases and understanding the phase transitions between them.<sup>8,12,20,22,23,32,33,239–243</sup> To penetrate at the nature of the magnetic properties of the materials, it is necessary to establish the symmetry properties and corresponding conservation laws of the microscopic models of magnetism. For ferromagnetic materials, the laws describing it are invariant under spatial rotations. Here, the order parameter is the magnetization, which measures the magnetic dipole density. Above the Curie temperature, the order parameter is zero, which is spatially invariant, and there is no symmetry breaking. Below the Curie temperature, however, the magnetization acquires a constant (in the idealized situation where we have full equilibrium; otherwise, translational symmetry gets broken as well) nonzero value which points in a certain direction. The residual rotational symmetries which leave the orientation of this vector invariant remain unbroken but the other rotations get spontaneously broken.

In the context of condensed matter physics, the qualitative explanations for the Goldstone theorem<sup>140–142</sup> is that for a Hamiltonian with a continuous symmetry many different degenerate ordered states can be realized (e.g., a Heisenberg ferromagnet in which all directions of the magnetization are possible). The collective mode with  $k \rightarrow 0$  describes a very slow transition of one such state to another (e.g., an extremely slow rotation of the total magnetization of the sample as a whole). Such a very slow variation of the magnetization should cost no energy and hence the dispersion curve  $E(k)$  starts from  $E = 0$  when  $k \rightarrow 0$ , i.e., there exists a gapless excitation. An important point is that for the Goldstone modes to appear,

the interactions need to be short ranged. In the so-called Lieb–Mattis modes,<sup>216</sup> the interactions between spins are effectively infinitely long ranged, as in the model a spin on a certain sublattice interacts with all spins on the other sublattice, independent of the “distance” between the spins. Thus there are no Goldstone modes in the Lieb–Mattis model<sup>216</sup> and the spin excitations are gapped. A physically more relevant example is the plasmon: the electromagnetic interactions are very long ranged, which leads to a gap in the excitation spectrum of bulk plasmons. It is possible to show that in a  $2D$  sheet of electrons, the dispersion  $E(k) \sim \sqrt{k}$ , thus in this case, the Coulomb interaction is not long ranged enough to induce a gap in the excitation spectrum. Also in the case of the breaking of gauge invariance, there is an important distinction between charge neutral systems, e.g., a Bose condensate of  $He^4$ , where there is a Goldstone mode called the Bogoliubov sound excitations,<sup>37</sup> whereas in a charge condensate, e.g., a superconductor, the elementary excitations are gapped due to the long range character of Coulomb interactions. These considerations on the elementary excitations in symmetry broken systems are important in order to establish whether or not long range order is possible at all.

The Goldstone theorem<sup>140–142</sup> states that, in a system with broken continuous symmetry (i.e., a system such that the ground state is not invariant under the operations of a continuous unitary group whose generators commute with the Hamiltonian), there exists a collective mode with frequency vanishing as the momentum goes to zero. For many-particle systems on a lattice, this statement needs a proper adaptation. In the above form, the Goldstone theorem is true only if the condensed and normal phases have the same translational properties. When translational symmetry is also broken, the Goldstone mode appears at zero frequency but at nonzero momentum, e.g., a crystal and a helical spin-density-wave (SDW) ordering.

All the four models considered above, the Heisenberg model, the Hubbard model, the Anderson and spin-fermion models, are spin rotationally invariant,  $\mathcal{R}H\mathcal{R}^\dagger = H$ . The spontaneous magnetization of the spin or fermion system on a lattice that possesses the spin rotational invariance, indicate on a broken symmetry effect, i.e., that the physical ground state is not an eigenstate of the time-independent generators of symmetry transformations on the original Hamiltonian of the system. As a consequence, there must exist an excitation mode that is an analog of the Goldstone mode for the continuous case (referred to as “massless” particles). It was shown that both the models, the Heisenberg model and the band or itinerant electron model of a solid, are capable of describing the theory of spin waves for ferromagnetic insulators and metals.<sup>238</sup> In their paper,<sup>244</sup> Herring and Kittel showed that in simple approximations, the spin waves can be described equally well in the framework of the model of localized spins or the model of itinerant electrons. Therefore the study of, for example, the temperature dependence of the average moment in magnetic transition metals in the framework of low-temperature spin-wave theory does not, as a rule, give any indications in favor of a particular



model. Moreover, the itinerant electron model (as well as the localized spin model) is capable of accounting for the exchange stiffness determining the properties of the transition region, known as the Bloch wall, which separates adjacent ferromagnetic domains with different directions of magnetization. The spin-wave stiffness constant  $D_{sw}$  is defined so<sup>241,244</sup> that the energy of a spin wave with a small wave vector  $\vec{q}$  is  $E \sim D_{sw}q^2$ . To characterize the dynamic behavior of the magnetic systems in terms of the quantum many-body theory, the generalized spin susceptibility (GSS) is a very useful tool.<sup>245</sup> The GSS is defined by

$$\chi(\vec{q}, \omega) = \int \langle\langle S_q^-(t), S_{-q}^+ \rangle\rangle \exp(-i\omega t) dt. \tag{9.21}$$

Here  $\langle\langle A(t), B \rangle\rangle$  is the retarded two-time temperature Green function<sup>37,217</sup> defined by

$$G^r = \langle\langle A(t), B(t') \rangle\rangle^r = -i\theta(t - t') \langle [A(t)B(t')]_\eta \rangle, \quad \eta = \pm 1, \tag{9.22}$$

where  $\langle \dots \rangle$  is the average over a grand canonical ensemble,  $\theta(t)$  is a step function, and square brackets represent the commutator or anticommutator

$$[A, B]_\eta = AB - \eta BA. \tag{9.23}$$

The Heisenberg representation is given by:

$$A(t) = \exp(iHt)A(0)\exp(-iHt). \tag{9.24}$$

For the Hubbard model  $S_i^- = a_{i\downarrow}^\dagger a_{i\uparrow}$ . This GSS satisfies the important sum rule

$$\int \text{Im}\chi(\vec{q}, \omega) d\omega = \pi(n_\downarrow - n_\uparrow) = -2\pi \langle S^z \rangle \tag{9.25}$$

It is possible to check that<sup>238</sup>

$$\chi(\vec{q}, \omega) = -\frac{2\langle S^z \rangle}{\omega} + \frac{q^2}{\omega^2} \left\{ \Psi(\vec{q}, \omega) - \frac{1}{q} \langle [Q_q^-, S_{-q}^+] \rangle \right\}. \tag{9.26}$$

Here the following notation was used for  $qQ_q^- = [S_q^-, H]$  and  $\Psi(\vec{q}, \omega) = \langle\langle Q_q^- | Q_{-q}^+ \rangle\rangle_\omega$ . It is clear from (9.25) that for  $q = 0$ , the GSS (9.26) contains only the first term corresponding to the spin-wave pole for  $q = 0$ , which exhausts the sum rule (9.25). For small  $q$ , due to the continuation principle, the GSS  $\chi(\vec{q}, \omega)$  must be dominated by the spin wave pole with the energy

$$\omega = Dq^2 = \frac{1}{2\langle S^z \rangle} \{ q \langle [Q_q^-, S_{-q}^+] \rangle - q^2 \lim_{\omega \rightarrow 0} \lim_{q \rightarrow 0} \Psi(\vec{q}, \omega) \} \tag{9.27}$$

This result is the direct consequence of the spin rotational invariance and is valid for all the four models considered above.

### 9.8. *Quantum protectorate and microscopic models of magnetism*

The main problem of the quantum theory of magnetism lies in choosing the most adequate microscopic model of magnetism of materials. The essence of this problem is related with the duality of localized and itinerant behavior of electrons. In describing of that duality, the microscopic theory meets the most serious difficulties.<sup>218</sup> This is the central issue of the quantum theory of magnetism.

The idea of quantum protectorate<sup>60</sup> reveals the essential difference in the behavior of the complex many-body systems at the low-energy and high-energy scales. There are many examples of the quantum protectorates.<sup>60</sup> According to this point of view, the nature of the underlying theory is unknowable until one raises the energy scale sufficiently to escape protection. The existence of two scales, the low-energy and high-energy scales, relevant to the description of magnetic phenomena was stressed by the author of this report in the papers<sup>218,219</sup> devoted to comparative analysis of localized and band models of quantum theory of magnetism. It was suggested by us<sup>219</sup> that the difficulties in the formulation of quantum theory of magnetism at the microscopic level, that are related to the choice of relevant models, can be understood better in the light of the quantum protectorate concept.<sup>219</sup> We argued that the difficulties in the formulation of adequate microscopic models of electron and magnetic properties of materials are intimately related to dual, **itinerant** and **localized** behavior of electrons. We formulated a criterion of what basic picture describes best this dual behavior. The main suggestion is that quasi-particle excitation spectra might provide distinctive signatures and good criteria for the appropriate choice of the relevant model. It was shown there,<sup>219</sup> that the low-energy spectrum of magnetic excitations in the magnetically-ordered solid bodies corresponds to a hydrodynamic pole ( $\vec{k}, \omega \rightarrow 0$ ) in the generalized spin susceptibility  $\chi$ , which is present in the Heisenberg, Hubbard, and the combined  $s$ - $d$  model. In the Stoner band model, the hydrodynamic pole is absent, there are no spin waves there. At the same time, the Stoner single-particle's excitations are absent in the Heisenberg model's spectrum. The Hubbard model with narrow energy bands contains both types of excitations: the collective spin waves (the low-energy spectrum) and Stoner single-particle's excitations (the high-energy spectrum). This is a big advantage and flexibility of the Hubbard model in comparison to the Heisenberg model. The latter, nevertheless, is a very good approximation to the realistic behavior in the limit  $\vec{k}, \omega \rightarrow 0$ , the domain where the hydrodynamic description is applicable, that is, for long wavelengths and low energies. The quantum protectorate concept was applied to the quantum theory of magnetism by the author of this report in the paper,<sup>219</sup> where a criterion of applicability of models of the quantum theory of magnetism to description of concrete substances was formulated. The criterion is based on the analysis of the model's low-energy and high-energy spectra.

## 10. Bogoliubov's Quasiaverages in Statistical Mechanics

Essential progress in the understanding of the spontaneously broken symmetry concept is connected with Bogoliubov's fundamental ideas of quasiaverages.<sup>37,66–68,99</sup> In the work of N. N. Bogoliubov "Quasiaverages in Problems of Statistical Mechanics" the innovative notion of *quasiaverage*<sup>66</sup> was introduced and applied to various problems of statistical physics. In particular, quasiaverages of Green's functions constructed from ordinary averages, degeneration of statistical equilibrium states, principle of weakened correlations, and particle pair states were considered. In this framework the  $1/q^2$ -type properties in the theory of the superfluidity of Bose and Fermi systems, the properties of basic Green functions for a Bose system in the presence of condensate, and a model with separated condensate were analyzed.

The method of quasiaverages is a constructive workable scheme for studying systems with spontaneous symmetry breakdown. A quasiaverage is a thermodynamic (in statistical mechanics) or vacuum (in quantum field theory) average of dynamical quantities in a specially modified averaging procedure, enabling one to take into account the effects of the influence of state degeneracy of the system. The method gives the so-called macro-objectivation of the degeneracy in the domain of quantum statistical mechanics and in quantum physics. In statistical mechanics, under spontaneous symmetry breakdown one can, by using the method of quasiaverages, describe macroscopic observable within the framework of the microscopic approach.

In considering problems of finding the eigenfunctions in quantum mechanics, it is well-known that the theory of perturbations should be modified substantially for the degenerate systems. In the problems of statistical mechanics, we always have the degenerate case due to existence of the additive conservation laws. The traditional approach to quantum statistical mechanics<sup>68,246</sup> is based on the unique canonical quantization of classical Hamiltonians for systems with finitely many degrees of freedom, together with the ensemble averaging in terms of traces involving a statistical operator  $\rho$ . For an operator  $\hat{A}$  corresponding to some physical quantity  $A$ , the average value of  $A$  will be given as

$$\langle A \rangle_H = \text{Tr} \rho A; \quad \rho = \exp^{-\beta H} / \text{Tr} \exp^{-\beta H} . \quad (10.1)$$

where  $H$  is the Hamiltonian of the system,  $\beta = 1/kT$  is the reciprocal of the temperature.

In general, the statistical operator<sup>69</sup> or density matrix  $\rho$  is defined by its matrix elements in the  $\varphi_m$ -representation:

$$\rho_{nm} = \frac{1}{N} \sum_{i=1}^N c_n^i (c_m^i)^* . \quad (10.2)$$

In this notation, the average value of  $A$  will be given as

$$\langle A \rangle = \frac{1}{N} \sum_{i=1}^N \int \Psi_i^* A \Psi_i d\tau . \quad (10.3)$$

The averaging in Eq. (10.3) is both over the state of the  $i$ th system and over all the systems in the ensemble. The Eq. (10.3) becomes

$$\langle A \rangle = \text{Tr } \rho A; \quad \text{Tr } \rho = 1. \quad (10.4)$$

Thus an ensemble of quantum mechanical systems is described by a density matrix.<sup>69</sup> In a suitable representation, a density matrix  $\rho$  takes the form

$$\rho = \sum_k p_k |\psi_k\rangle \langle \psi_k|$$

where  $p_k$  is the probability of a system chosen at random from the ensemble will be in the microstate  $|\psi_k\rangle$ . So the trace of  $\rho$ , denoted by  $\text{Tr}(\rho)$ , is unity. This is the quantum mechanical analogue of the fact that the accessible region of the classical phase space has total probability of unity. It is also assumed that the ensemble in question is stationary, i.e., it does not change in time. Therefore, by Liouville theorem,  $[\rho, H] = 0$ , i.e.,  $\rho H = H\rho$  where  $H$  is the Hamiltonian of the system. Thus the density matrix describing  $\rho$  is diagonal in the energy representation.

Suppose that

$$H = \sum_i E_i |\psi_i\rangle \langle \psi_i|$$

where  $E_i$  is the energy of the  $i$ th energy eigenstate. If a system  $i$ th energy eigenstate has  $n_i$  number of particles, the corresponding observable, the number operator, is given by

$$N = \sum_i n_i |\psi_i\rangle \langle \psi_i|.$$

It is known,<sup>69</sup> that the state  $|\psi_i\rangle$  has (unnormalized) probability

$$p_i = e^{-\beta(E_i - \mu n_i)}.$$

Thus the grand canonical ensemble is the mixed state

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| = \sum_i e^{-\beta(E_i - \mu n_i)} |\psi_i\rangle \langle \psi_i| = e^{-\beta(H - \mu N)}. \quad (10.5)$$

The grand partition, the normalizing constant for  $\text{Tr}(\rho)$  to be unity, is

$$\mathcal{Z} = \text{Tr}[e^{-\beta(H - \mu N)}].$$

Thus we obtain<sup>69</sup>

$$\langle A \rangle = \text{Tr } \rho A = \text{Tr } e^{\beta(\Omega - H + \mu N)} A. \quad (10.6)$$

Here  $\beta = 1/k_B T$  is the reciprocal temperature and  $\Omega$  is the normalization factor.

It is known<sup>69</sup> that the averages  $\langle A \rangle$  are unaffected by a change of representation. The most important is the representation in which  $\rho$  is diagonal  $\rho_{mn} = \rho_m \delta_{mn}$ . We then have  $\langle \rho \rangle = \text{Tr } \rho^2 = 1$ . It is clear then that  $\text{Tr } \rho^2 \leq 1$  in any representation. The core of the problem lies in establishing the existence of a thermodynamic limit

(such as  $N/V = \text{const}$ ,  $V \rightarrow \infty$ ,  $N = \text{number of degrees of freedom}$ ,  $V = \text{volume}$ ) and its evaluation for the quantities of interest.

The evolution equation for the density matrix is a quantum analog of the Liouville equation in classical mechanics. A related equation describes the time evolution of the expectation values of observables; it is given by the Ehrenfest theorem. Canonical quantization yields a quantum-mechanical version of this theorem. This procedure, often used to devise quantum analogues of classical systems, involves describing a classical system using Hamiltonian mechanics. Classical variables are then re-interpreted as quantum operators, while Poisson brackets are replaced by commutators. In this case, the resulting equation is

$$\frac{\partial}{\partial t} \rho = -\frac{i}{\hbar} [H, \rho], \quad (10.7)$$

where  $\rho$  is the density matrix. When applied to the expectation value of an observable, the corresponding equation is given by Ehrenfest theorem, and takes the form

$$\frac{d}{dt} \langle A \rangle = \frac{i}{\hbar} \langle [H, A] \rangle, \quad (10.8)$$

where  $A$  is an observable. Thus in the statistical mechanics, the average  $\langle A \rangle$  of any dynamical quantity  $A$  is defined in a single-valued way.

In the situations with degeneracy, the specific problems appear. In quantum mechanics, if two linearly independent state vectors (wavefunctions in the Schrodinger picture) have the same energy, there is a degeneracy.<sup>247</sup> In this case, more than one independent state of the system corresponds to a single energy level. If the statistical equilibrium state of the system possesses lower symmetry than the Hamiltonian of the system (i.e., the situation with the spontaneous symmetry breakdown), then it is necessary to supplement the averaging procedure (10.6) by a rule forbidding irrelevant averaging over the values of macroscopic quantities considered for which a change is not accompanied by a change in energy.

This is achieved by introducing quasiaverages, that is, averages over the Hamiltonian  $H_{\nu\vec{e}}$  supplemented by infinitesimally-small terms that violate the additive conservations laws  $H_{\nu\vec{e}} = H + \nu(\vec{e} \cdot \vec{M})$ , ( $\nu \rightarrow 0$ ). Thermodynamic averaging may turn out to be unstable with respect to such a change of the original Hamiltonian, which is another indication of degeneracy of the equilibrium state.

According to Bogoliubov,<sup>66</sup> the quasiaverage of a dynamical quantity  $A$  for the system with the Hamiltonian  $H_{\nu\vec{e}}$  is defined as the limit

$$\asymp A \asymp = \lim_{\nu \rightarrow 0} \langle A \rangle_{\nu\vec{e}}, \quad (10.9)$$

where  $\langle A \rangle_{\nu\vec{e}}$  denotes the ordinary average taken over the Hamiltonian  $H_{\nu\vec{e}}$ , containing the small symmetry-breaking terms introduced by the inclusion parameter  $\nu$ , which vanish as  $\nu \rightarrow 0$  after passage to the thermodynamic limit  $V \rightarrow \infty$ . Thus, the existence of degeneracy is reflected directly in the quasiaverages by their

dependence upon the arbitrary unit vector  $\vec{e}$ . It is also clear that

$$\langle A \rangle = \int \Re A \Im d\vec{e}. \tag{10.10}$$

According to definition (10.10), the ordinary thermodynamic average is obtained by extra averaging of the quasiaverage over the symmetry-breaking group. Thus to describe the case of a degenerate state of statistical equilibrium quasiaverages are more convenient, more physical, than ordinary averages.<sup>68,246</sup> The latter are the same quasiaverages only averaged over all the directions  $\vec{e}$ .

It is necessary to stress that the starting point for Bogoliubov’s work<sup>66</sup> was an investigation of additive conservation laws and selection rules, continuing and developing the approach by P. Curie for derivation of selection rules for physical effects. Bogoliubov demonstrated that in the cases when the state of statistical equilibrium is degenerate, as in the case of the Heisenberg ferromagnet (9.5), one can remove the degeneracy of equilibrium states with respect to the group of spin rotations by including in the Hamiltonian  $H$  an additional noninvariant term  $\nu M_z V$  with an infinitely small  $\nu$ . Thus the quasiaverages do not follow the same selection rules as those which govern the ordinary averages. For the Heisenberg ferromagnet, the ordinary averages must be invariant with regard to the spin rotation group. The corresponding quasiaverages possess only the property of covariance. It is clear that the unit vector  $\vec{e}$ , i.e., the direction of the magnetization  $\vec{M}$  vector, characterizes the degeneracy of the considered state of statistical equilibrium. In order to remove the degeneracy one should fix the direction of the unit vector  $\vec{e}$ . It can be chosen to be along the  $z$  direction. Then all the quasiaverages will be the definite numbers. This is the kind that one usually deals with in the theory of ferromagnetism.

The value of the quasi-average (10.9) may depend on the concrete structure of the additional term  $\Delta H = H_\nu - H$ , if the dynamical quantity to be averaged is not invariant with respect to the symmetry group of the original Hamiltonian  $H$ . For a degenerate state, the limit of ordinary averages (10.10) as the inclusion parameters  $\nu$  of the sources tend to zero in an arbitrary fashion, may not exist. For a complete definition of quasiaverages it is necessary to indicate the manner in which these parameters tend to zero in order to ensure convergence.<sup>248</sup> On the other hand, in order to remove degeneracy it suffices, in the construction of  $H$ , to violate only those additive conservation laws whose switching lead to instability of the ordinary average. Thus in terms of quasiaverages, the selection rules for the correlation functions<sup>68,249</sup> that are not relevant are those that are restricted by these conservation laws.

By using  $H_\nu$ , we define the state  $\omega(A) = \langle A \rangle_\nu$  and then let  $\nu$  tend to zero (after passing to the thermodynamic limit). If all averages  $\omega(A)$  get infinitely small increments under infinitely small perturbations  $\nu$ , this means that the state of statistical equilibrium under consideration is nondegenerate.<sup>68,249</sup> However, if some states have finite increments as  $\nu \rightarrow 0$ , then the state is degenerate. In this case, instead of ordinary averages  $\langle A \rangle_H$ , one should introduce the quasiaverages (10.9), for which the usual selection rules do not hold.

The method of quasiaverages is directly related to the principle weakening of the correlation<sup>68,249</sup> in many-particle systems. According to this principle, the notion of the weakening of the correlation, known in statistical mechanics,<sup>37,68</sup> in the case of state degeneracy must be interpreted in the sense of the quasiaverages.<sup>249</sup>

The quasiaverages may be obtained from the ordinary averages by using the cluster property which was formulated by Bogoliubov.<sup>249</sup> This was first done when deriving the Boltzmann equations from the chain of equations for distribution functions, and in the investigation of the model Hamiltonian in the theory of superconductivity.<sup>37,66-68,99</sup> To demonstrate this let us consider averages (quasiaverages) of the form

$$F(t_1, x_1, \dots, t_n, x_n) = \langle \dots \Psi^\dagger(t_1, x_1) \dots \Psi(t_j, x_j) \dots \rangle, \tag{10.11}$$

where the number of creation operators  $\Psi^\dagger$  may not be equal to the number of annihilation operators  $\Psi$ . We fix times and split the arguments  $(t_1, x_1, \dots, t_n, x_n)$  into several clusters  $(\dots, t_\alpha, x_\alpha, \dots), \dots, (\dots, t_\beta, x_\beta, \dots)$ . Then it is reasonable to assume that the distances between all clusters  $|x_\alpha - x_\beta|$  tend to infinity. Then, according to the cluster property, the average value (10.11) tends to the product of averages of collections of operators with the arguments  $(\dots, t_\alpha, x_\alpha, \dots), \dots, (\dots, t_\beta, x_\beta, \dots)$

$$\lim_{|x_\alpha - x_\beta| \rightarrow \infty} F(t_1, x_1, \dots, t_n, x_n) = F(\dots, t_\alpha, x_\alpha, \dots) \dots F(\dots, t_\beta, x_\beta, \dots). \tag{10.12}$$

For equilibrium states with small densities and short-range potential, the validity of this property can be proven.<sup>68</sup> For the general case, the validity of the cluster property has not yet been proved. Bogoliubov formulated it not only for ordinary averages but also for quasiaverages, i.e., for anomalous averages, too. It works for many important models, including the models of superfluidity and superconductivity.

To illustrate this statement, consider Bogoliubov's theory of a Bose-system with separated condensate, which is given by the Hamiltonian<sup>37,68</sup>

$$\begin{aligned} H_\Lambda &= \int_\Lambda \Psi^\dagger(x) \left( -\frac{\Delta}{2m} \right) \Psi(x) dx - \mu \int_\Lambda \Psi^\dagger(x) \Psi(x) dx \\ &+ \frac{1}{2} \int_{\Lambda^2} \Psi^\dagger(x_1) \Psi^\dagger(x_2) \Phi(x_1 - x_2) \Psi(x_2) \Psi(x_1) dx_1 dx_2. \end{aligned} \tag{10.13}$$

This Hamiltonian can also be written in the following form

$$\begin{aligned} H_\Lambda &= H_0 + H_1 \\ &= \int_\Lambda \Psi^\dagger(q) \left( -\frac{\Delta}{2m} \right) \Psi(q) dq \\ &+ \frac{1}{2} \int_{\Lambda^2} \Psi^\dagger(q) \Psi^\dagger(q') \Phi(q - q') \Psi(q') \Psi(q) dq dq'. \end{aligned} \tag{10.14}$$

Here,  $\Psi(q)$ , and  $\Psi^\dagger(q)$  are the operators of annihilation and creation of bosons. They satisfy the canonical commutation relations

$$[\Psi(q), \Psi^\dagger(q')] = \delta(q - q'); \quad [\Psi(q), \Psi(q')] = [\Psi^\dagger(q), \Psi^\dagger(q')] = 0. \quad (10.15)$$

The system of bosons is contained in the cube  $A$  with the edge  $L$  and volume  $V$ . It was assumed that it satisfies periodic boundary conditions and the potential  $\Phi(q)$  is spherically symmetric and proportional to the small parameter. It was also assumed that, at temperature zero, a certain macroscopic number of particles having a nonzero density is situated in the state with momentum zero.

The operators  $\Psi(q)$ , and  $\Psi^\dagger(q)$  are represented in the form

$$\Psi(q) = a_0/\sqrt{V}; \quad \Psi^\dagger(q) = a_0^\dagger/\sqrt{V}, \quad (10.16)$$

where  $a_0$  and  $a_0^\dagger$  are the operators of annihilation and creation of particles with momentum zero.

To explain the phenomenon of superfluidity, one should calculate the spectrum of the Hamiltonian, which is quite a difficult problem. Bogoliubov suggested the idea of approximate calculation of the spectrum of the ground state and its elementary excitations based on the physical nature of superfluidity. His idea consists of a few assumptions. The main assumption is that at temperature zero, the macroscopic number of particles (with nonzero density) has the momentum zero. Therefore, in the thermodynamic limit, the operators  $a_0/\sqrt{V}$  and  $a_0^\dagger/\sqrt{V}$  commute

$$\lim_{V \rightarrow \infty} [a_0/\sqrt{V}, a_0^\dagger/\sqrt{V}] = \frac{1}{V} \rightarrow 0 \quad (10.17)$$

and are  $c$ -numbers. Hence, the operator of the number of particles  $N_0 = a_0^\dagger a_0$  is a  $c$ -number, too. It is worth noting that the Hamiltonian (10.14) is invariant under the gauge transformation  $\tilde{a}_k = \exp(i\varphi)a_k$ ,  $\tilde{a}_k^\dagger = \exp(-i\varphi)a_k^\dagger$ , where  $\varphi$  is an arbitrary real number. Therefore, the averages  $\langle a_0/\sqrt{V} \rangle$  and  $\langle a_0^\dagger/\sqrt{V} \rangle$  must vanish. But this contradicts to the assumption that  $a_0/\sqrt{V}$  and  $a_0^\dagger/\sqrt{V}$  must become  $c$ -numbers in the thermodynamic limit. In addition it must be taken into account that  $a_0^\dagger a_0/V = N_0/V \neq 0$  which implies that  $a_0/\sqrt{V} = N_0 \exp(i\alpha)/\sqrt{V} \neq 0$  and  $a_0^\dagger/\sqrt{V} = N_0 \exp(-i\alpha)/\sqrt{V} \neq 0$ , where  $\alpha$  is an arbitrary real number. This contradiction may be overcome if we assume that the eigenstates of the Hamiltonian are degenerate and not invariant under gauge transformations, i.e., that a spontaneous breaking of symmetry takes place.

Thus the averages  $\langle a_0/\sqrt{V} \rangle$  and  $\langle a_0^\dagger/\sqrt{V} \rangle$ , which are nonzero under spontaneously broken gauge invariance, are called anomalous averages or *quasiaverages*. This innovative idea of Bogoliubov penetrates deeply into the modern quantum physics. The systems with spontaneously broken symmetry are studied by use of the transformation of the operators of the form

$$\Psi(q) = a_0/\sqrt{V} + \theta(q); \quad \Psi^\dagger(q) = a_0^\dagger/\sqrt{V} + \theta^*(q), \quad (10.18)$$



where  $a_0/\sqrt{V}$  and  $a_0^\dagger/\sqrt{V}$  are the numbers first introduced by Bogoliubov in 1947 in his investigation of the phenomenon of superfluidity.<sup>37,66,68,250</sup> The main conclusion was made that for the systems with spontaneously broken symmetry, the quasiaverages should be studied instead of the ordinary averages. It turns out that the long-range order appears not only in the system of Bose-particles but also in all systems with spontaneously broken symmetry. Bogoliubov's papers outlined above anticipated the methods of investigation of systems with spontaneously broken symmetry for many years.

As mentioned above, in order to explain the phenomenon of superfluidity, Bogoliubov assumed that the operators  $a_0/\sqrt{V}$  and  $a_0^\dagger/\sqrt{V}$  become  $c$ -numbers in the thermodynamic limit. This statement was rigorously proved in the papers by Bogolyubov and some other authors. Bogolyubov's proof was based on the study of the equations for two-time Green's functions and on the assumption that the cluster property holds. It was proved that the solutions of equations for Green's functions for the system with Hamiltonian (10.14) coincide with the solutions of the equations for the system with the same Hamiltonian in which the operators  $a_0/\sqrt{V}$  and  $a_0^\dagger/\sqrt{V}$  are replaced by numbers. These numbers should be determined from the condition of minimum for free energy. Since all the averages in both systems coincide, their free energies coincide, too.

It is worth noting that the validity of the replacement of the operators  $a_0$  and  $a_0^\dagger$  by  $c$ -numbers in the thermodynamic limit was confirmed in the numerous subsequent publications of various authors.<sup>251-253</sup> Lieb, Seiringer and Yngvason<sup>252</sup> analyzed justification of  $c$ -number substitutions in bosonic Hamiltonians. The validity of substituting a  $c$ -number  $z$  for the  $k = 0$  mode operator  $a_0$  was established rigorously in full generality, thereby verifying that aspect of Bogoliubov's 1947 theory. The authors show that this substitution not only yields the correct value of thermodynamic quantities such as the pressure or ground state energy, but also the value of  $|z|^2$  that maximizes the partition function equals the true amount of condensation in the presence of a gauge-symmetry-breaking term. This point had previously been elusive. Thus Bogoliubov's 1947 analysis of the many-body Hamiltonian by means of a  $c$ -number substitution for the most relevant operators in the problem, the zero-momentum mode operators, was justified rigorously. Since the Bogoliubov's 1947 analysis is one of the key developments in the theory of the Bose gas, especially the theory of the low density gases currently at the forefront of experiment, this result is of importance for the legitimation of that theory. Additional arguments were given in Ref. 253, where the Bose-Einstein condensation and spontaneous  $U(1)$  symmetry breaking were investigated. Based on Bogoliubov's truncated Hamiltonian  $H_B$  for a weakly interacting Bose system, and adding a  $U(1)$  symmetry breaking term  $\sqrt{V}(\lambda a_0 + \lambda^* a_0^\dagger)$  to  $H_B$ , authors show that by using the coherent state theory and the mean-field approximation rather than the  $c$ -number approximations, the Bose-Einstein condensation occurs if and only if the  $U(1)$  symmetry of the system is spontaneously broken. The real ground state energy and the justification

of the Bogoliubov  $c$ -number substitution were given by solving the Schroedinger eigenvalue equation and using the self-consistent condition. Thus the Bogoliubov  $c$ -number substitutions were fully correct and the symmetry breaking causes the displacement of the condensate state.

The concept of quasiaverages was introduced by Bogoliubov on the basis of an analysis of many-particle systems with a degenerate statistical equilibrium state. Such states are inherent to various physical many-particle systems.<sup>37,68</sup> Those are liquid helium in the superfluid phase, metals in the superconducting state, magnets in the ferromagnetically ordered state, liquid crystal states, the states of superfluid nuclear matter, etc. (for a review, see Refs. 218 and 254). In the case of superconductivity, the source

$$\nu \sum_k v(k)(a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger + a_{-k\downarrow} a_{k\uparrow})$$

was inserted in the BCS-Bogoliubov Hamiltonian, and the quasiaverages were defined by use of the Hamiltonian  $H_\nu$ . In the general case, the sources are introduced to remove degeneracy. If infinitesimal sources give infinitely small contributions to the averages, then this means that the corresponding degeneracy is absent, and there is no reason to insert sources in the Hamiltonian. Otherwise, the degeneracy takes place, and it is removed by the sources. The ordinary averages can be obtained from quasiaverages by averaging with respect to the parameters that characterize the degeneracy.

N. N. Bogoliubov, Jr.<sup>248</sup> considered some features of quasiaverages for model systems with four-fermion interaction. He discussed the treatment of certain three-dimensional model systems which can be solved exactly. For this aim, a new effective way of defining quasiaverages for the systems under consideration was proposed.

Peletminskii and Sokolovskii<sup>255</sup> have found general expressions for the operators of the flux densities of physical variables in terms of the density operators of these variables. The method of quasiaverages and the expressions found for the flux operators were used to obtain the averages of these operators in terms of the thermodynamic potential in a state of statistical equilibrium of a superfluid liquid.

Vozyakov<sup>256</sup> reformulated the theory of quantum crystals in terms of quasiaverages. He analyzed a Bose system with periodic distribution of particles which simulates an ensemble in which the particles cannot be regarded as vibrating independently about a position of equilibrium lattice sites. With allowance for macroscopic filling of the states corresponding to the distinguished symmetry, a calculation was made of an excitation spectrum in which there exists a collective branch of gapless type.

Peregoudov<sup>257</sup> discussed the effective potential method, used in quantum field theory to study spontaneous symmetry breakdown, from the point of view of Bogoliubov's quasiaveraging procedure. It was shown that the effective potential method is a disguised type of this procedure. The catastrophe theory approach to the study of phase transitions was discussed and the existence of the potentials used in that

approach was proved from the statistical point of view. It was shown that in the case of broken symmetry, the nonconvex effective potential is not a Legendre transform of the generating functional for connected Green's functions. Instead, it is a part of the potential used in catastrophe theory. The relationship between the effective potential and the Legendre transform of the generating functional for connected Green's functions is given by Maxwell's rule. A rigorous rule for evaluating quasiaveraged quantities within the framework of the effective potential method was established.

N. N. Bogoliubov, Jr. with M. Yu. Kovalevsky and co-authors<sup>258</sup> developed a statistical approach for solving the problem of classification of equilibrium states in condensed media with spontaneously broken symmetry based on the quasiaverage concept. Classification of equilibrium states of condensed media with spontaneously broken symmetry was carried out. The generators of residual and spatial symmetries were introduced and equations of classification for the order parameter has been found. Conditions of residual symmetry and spatial symmetry were formulated. The connection between these symmetry conditions and equilibrium states of various media with tensor order parameter was found out. An analytical solution of the problem of classification of equilibrium states for superfluid media, liquid crystals and magnets with tensor order parameters was obtained. Superfluid  ${}^3\text{He}$ , liquid crystals, quadrupolar magnetics were considered in detail. Possible homogeneous and heterogeneous states were found out. Discrete and continuous thermodynamic parameters, which define an equilibrium state, allowable form of order parameter, residual symmetry, and spatial symmetry generators were established. This approach, which is an alternative to the well-known Ginzburg–Landau method, does not contain any model assumptions concerning the form of the free energy as functional of the order parameter and does not employ the requirement of temperature closeness to the point of phase transition. For all investigated cases, they found the structure of the order parameters and the explicit forms of generators of residual and spatial symmetries. Under certain restrictions, they established the form of the order parameters in case of spins 0, 1/2, 1 and proposed the physical interpretation of the studied degenerate states of condensed media.

To summarize, the Bogoliubov's quasiaverages concept plays an important role in equilibrium statistical mechanics of many-particle systems. According to that concept, infinitely small perturbations can trigger macroscopic responses in the system if they break some symmetry and remove the related degeneracy (or quasidegeneracy) of the equilibrium state. As a result, they can produce macroscopic effects even when the perturbation magnitude is tend to zero, provided that happens after passing to the thermodynamic limit.

### 10.1. *Bogoliubov theorem on the singularity of $1/q^2$*

Spontaneous symmetry breaking in a nonrelativistic theory is manifested in a nonvanishing value of a certain macroscopic parameter (spontaneous polarization, density

of a superfluid component, etc.). In this sense it is intimately related to the problem of phase transitions. These problems were discussed intensively from different points of view in literature.<sup>37,66,68,259</sup> In particular, there has been an extensive discussion of the conjecture that the spontaneous symmetry breaking corresponds under a certain restriction on the nature of the interaction to a branch of collective excitations of zero-gap type ( $\lim_{q \rightarrow 0} E(q) = 0$ ). It was shown in the previous sections that some ideas here have been borrowed from the theory of elementary particles, in which the ground state (vacuum) is noninvariant under a group of continuous transformations that leave the field equations invariant, and the transition from one vacuum to the other can be described in terms of the excitation of an infinite number of zero-mass particles (Goldstone bosons).

It should be stressed here that the main questions of this kind have already been resolved by Bogoliubov in his paper<sup>66</sup> on models of Bose and Fermi systems of many particles with a gauge-invariant interaction. Reference 259 reproduces the line of arguments of the corresponding section in Ref. 66, in which the inequality for the mass operator  $M$  of a boson system, which is expressed in terms of “normal” and “anomalous” Green’s functions, made it possible, under the assumption of its regularity for  $E = 0$  and  $q = 0$ , to obtain “acoustic” nature of the energy of the low-lying excitation ( $E = \sqrt{sq}$ ). It is also noted in Ref. 66 that a “gap” in the spectrum of elementary excitations may be due either to a discrepancy in the approximations that are used (for the mass operator and the free energy) or to a certain choice of the interaction potential, (i.e., essentially to an incorrect use of quasiaverages). This Bogoliubov’s remark is still important, especially in connection with the application of different model Hamiltonians to concrete systems.

It was demonstrated above that Bogoliubov’s fundamental concept of quasiaverages is an effective method of investigating problems related to degeneracy of a state of statistical equilibrium due to the presence of additive conservation laws or alternatively invariance of the Hamiltonian of the system under a certain group of transformations. The mathematical apparatus of the method of quasi-averages includes the Bogoliubov theorem<sup>37,66,68</sup> on singularities of type  $1/q^2$  and the Bogoliubov inequality for Green and correlation functions as a direct consequence of the method. It includes algorithms for establishing non-trivial estimates for equilibrium quasiaverages, enabling one to study the problem of ordering in statistical systems and to elucidate the structure of the energy spectrum of the underlying excited states. In that sense the mathematical scheme proposed by Bogoliubov<sup>37,66,68</sup> is a workable tool for establishing nontrivial inequalities for equilibrium mean values (quasiaverages) for the commutator Green’s functions and also the inequalities that majorize it. Those inequalities enable one to investigate questions relating to the specific ordering in models of statistical mechanics and to consider the structure of the energy spectrum of low-lying excited states in the limit ( $q \rightarrow 0$ ).

Let us consider the proof of Bogoliubov’s theorem on singularities of  $1/q^2$ -type. For this aim consider the retarded, advanced, and causal Green’s functions of the

following form<sup>37,66,68,218,219</sup>

$$G^r(A, B; t - t') = \langle\langle A(t), B(t') \rangle\rangle^r = -i\theta(t - t')\langle[A(t), B(t')]_\eta\rangle, \eta = \pm, \quad (10.19)$$

$$G^a(A, B; t - t') = \langle\langle A(t), B(t') \rangle\rangle^a = i\theta(t' - t)\langle[A(t), B(t')]_\eta\rangle, \eta = \pm, \quad (10.20)$$

$$\begin{aligned} G^c(A, B; t - t') &= \langle\langle A(t), B(t') \rangle\rangle^c = iT\langle A(t)B(t') \rangle \\ &= i\theta(t - t')\langle A(t)B(t') \rangle + \eta i\theta(t' - t)\langle B(t')A(t) \rangle, \eta = \pm. \end{aligned} \quad (10.21)$$

It is well-known<sup>37,66,68,218,219</sup> that the Fourier transforms of the retarded and advanced Green's functions are different limiting values (on the real axis) of the same function that is holomorphic on the complex  $\mathcal{E}$ -plane with cuts along the real axis

$$\langle\langle A|B \rangle\rangle_{\mathcal{E}} = \int_{-\infty}^{+\infty} d\omega \frac{J(B, A; \omega)(\exp(\beta\omega) - \eta)}{\mathcal{E} - \omega}. \quad (10.22)$$

Here, the function  $J(B, A; \omega)$  possesses the properties

$$J(A^\dagger, A; \omega) \geq 0; \quad J^*(B, A; \omega) = J(A^\dagger, B^\dagger; \omega). \quad (10.23)$$

Moreover, it is a bilinear form of the operators  $A = A(0)$  and  $B = B(0)$ . This implies that the bilinear form

$$-\langle\langle A|B \rangle\rangle_{\mathcal{E}} = Z(A, B) = \int_{-\infty}^{+\infty} d\omega \frac{J(B, A; \omega)(\exp(\beta\omega) - \eta)}{\omega} \quad (10.24)$$

possesses the similar properties

$$Z(A, A^\dagger) \geq 0; \quad Z^*(A, B) = Z(B^\dagger, A^\dagger). \quad (10.25)$$

Therefore, the bilinear form  $Z(A, B)$  possesses all properties of the scalar product<sup>68</sup> in linear space whose elements are operators  $A, B, \dots$  that act in the Fock space of states. This scalar product can be introduced as follows:

$$(A, B) = Z(A^\dagger, B). \quad (10.26)$$

Just as this is proved for the scalar product in a Hilbert space,<sup>68</sup> we can establish the inequality

$$|(A, B)|^2 \leq (A, A^\dagger)(B^\dagger, B). \quad (10.27)$$

This implies that  $(A, B) = 0$  if  $(A, A) = 0$  or  $(B, B) = 0$ . If we introduce a factor-space with respect to the collection of the operators for which  $(A, A) = 0$ , then we obtain an ordinary Hilbert space whose elements are linear operators, and the scalar product is given by (10.26).

To illustrate this line of reasoning, consider Bogoliubov's theory of a Bose-system with separated condensate,<sup>37,68</sup> which is given by the Hamiltonian (10.14) in the system with separated condensate, the anomalous averages  $\langle a_0/\sqrt{V} \rangle$  and  $\langle a_0^\dagger/\sqrt{V} \rangle$  are nonzero. This indicates that the states of the Hamiltonian are degenerate with

respect to the number of particles. In order to remove this degeneracy, Bogoliubov inserted infinitesimal terms of the form  $\nu\sqrt{V}(a_0 + a_0^\dagger)$  in the Hamiltonian. As a result, we obtain the Hamiltonian

$$H_\nu = H - \nu\sqrt{V}(a_0 + a_0^\dagger). \tag{10.28}$$

For this Hamiltonian, the fundamental theorem “on singularities of  $1/q^2$ -type” was proved for Green’s functions.<sup>37,66,68,259</sup> In its simplest version, this theorem consists of the fact that the Fourier components of the Green’s functions corresponding to energy  $E = 0$  satisfy the inequality

$$|\langle\langle a_q, a_q^\dagger \rangle\rangle_{E=0}| \geq \frac{\text{const}}{q^2} \quad \text{as } q^2 \rightarrow 0. \tag{10.29}$$

Here  $\langle\langle a_q, a_q^\dagger \rangle\rangle_{E=0}$  is the two-time temperature commutator Green function in the energy representation, and  $a_q^\dagger, a_q$  are the creation and annihilation operators of a particle with momentum  $\vec{q}$ . A more detailed consideration gives the following result<sup>37,66,68,259</sup>

$$\begin{aligned} \langle\langle a_q, a_q^\dagger \rangle\rangle_{E=0} &\geq \frac{N_0}{4\pi \left( N \frac{q^2}{2m} + \nu N_0 V^{1/2} \right)} \\ &= \frac{N_0 2m}{4\pi (Nq^2 + \nu 2m N_0 V^{1/2})} \\ &= \frac{\rho_0 m}{4\pi (\rho q^2 + \nu 2m \sqrt{\rho_0})}, \\ \frac{N}{V} = \rho, \quad \frac{N_0}{V} = \rho_0. \end{aligned} \tag{10.30}$$

Finally, by passing here to the limit as  $\nu \rightarrow 0$ , we obtain the required inequality

$$\langle\langle a_q, a_q^\dagger \rangle\rangle_{E=0} \geq \frac{\rho_0 m}{4\pi \rho} \frac{1}{q^2}. \tag{10.31}$$

The concept of quasiaverages is indirectly related to the theory of phase transition. The instability of thermodynamic averages with respect to perturbations of the Hamiltonian by a breaking of the invariance with respect to a certain group of transformations means that in the system, transition to an extremal state occurs. In quantum field theory, for a number of model systems, it has been proven that there is a phase transition, and the validity of the Bogolyubov theorem on singularities of type  $1/q^2$  has been established.<sup>37,66,68</sup> In addition, the possibility has been investigated of local instability of the vacuum and the appearance of a changed structure in it.

In summary, the main achievement of the method of quasiaverages is the fundamental Bogoliubov theorem<sup>37,66,68,259</sup> on the singularity of  $1/q^2$  for Bose and Fermi systems with gauge-invariant interaction between particles. The singularities in the Green functions specified in Bogoliubov’s theorem which appear when corresponding to elementary excitations in the physical system under study. Bogoliubov’s

theorem also predicts the asymptotic behavior for small momenta of macroscopic properties of the system which are connected with Green functions by familiar theorems. The theorem establishes the asymptotic behavior of Green functions in the limit of small momenta ( $q \rightarrow 0$ ) for systems of interacting particles in the case of a degenerate statistical equilibrium state.

The appearance of singularities in the Green functions as ( $q \rightarrow 0$ ) is connected with the presence of a branch of collective excitations in the energy spectrum of the system that corresponds with spontaneous symmetry breaking under certain restrictions on the interaction potential.

The nature of the energy spectrum of elementary excitations may be studied with the aid of the mass (or self-energy) operator  $M$  inequality constructed for Green functions of type (10.29). In the case of Bose systems, for a finite temperature, this inequality has the form:

$$|M_{11}(0, q) - M_{12}(0, q)| \leq \frac{\text{const}}{q^2}. \quad (10.32)$$

For ( $q = 0$ ), formula (10.31) yields a generalization of the so-called Hugenholtz-Pines formula<sup>260</sup> to finite temperatures. If one assumes that the mass operator is regular in a neighbourhood of the point ( $E = 0, q = 0$ ), then one can use (10.29) to prove the absence of a gap in the (phonon-type) excitation energy spectrum.

In the case of zero temperatures, the inequality (10.31) establishes a connection between the density of the continuous distribution of the particle momenta and the minimum energy of an excited state. Relations of type (10.31) should also be valid in quantum field theory, in which a spontaneous symmetry breaking (at a transition between two ground states) results in an infinite number of particles of zero mass (Goldstone's theorem), which are interpreted as singularities for small momenta in the quantum field Green functions. Bogoliubov's theorem has been applied to numerous statistical and quantum-field-theoretical models with a spontaneous symmetry breaking. In particular, S. Takada<sup>261</sup> investigated the relation between the long-range order in the ground state and the collective mode, namely, the Goldstone particle, on the basis of Bogoliubov's  $1/q^2$  theorem. It was pointed out that Bogoliubov's inequality rules out the long-range orders in the ground states of the isotropic Heisenberg model, the half-filled Hubbard model and the interacting Bose system for one dimension while it admits the long-range orders for two dimensions. Takada's proof was based on the fact that the lowest-excited state that can be regarded as the Goldstone particle that has the energy  $E(q) \propto |q|$  for small  $q$ . This energy spectrum was exactly given in the one-dimensional models and was shown to be proven in the ordered state on a reasonable assumption except for the ferromagnetic case. Baryakhtar and Yablonsky<sup>262</sup> applied Bogoliubov's theorem on  $1/q^2$  law to quantum theory of magnetism and studied the asymptotic behavior of the correlation functions of magnets in the long-wavelength limit.

These papers and also some others demonstrated the strength of the  $1/q^2$  theorem for obtaining rigorous proofs of the absence of specific ordering in one- and

two-dimensional systems, in which spontaneous symmetry is broken in completely different ways: ferro-ferri-, and antiferromagnets, systems that exhibit superfluidity and superconductivity, etc. All that indicates that  $1/q^2$  theorem provides the workable and very useful tool for rigorous investigation of the problem of specific ordering in various concrete systems of interacting particles.

**10.2. Bogoliubov’s inequality and the Mermin-Wagner theorem**

One of the most interesting features of an interacting system is the existence of a macroscopic order which breaks the underlying symmetry of the Hamiltonian. It was shown above, that the continuous rotational symmetry (in three-dimensional spin space) of the isotropic Heisenberg ferromagnet is broken by the spontaneous magnetization that exists in the limit of vanishing magnetic field for a three-dimensional lattice. For systems of restricted dimensionality, it has been argued long ago that there is no macroscopic order, on the basis of heuristic arguments. For instance, because the excitation spectrum for systems with continuous symmetry has no gap, the integral of the occupation number over momentum will diverge in one and two dimensions for any nonzero temperature. The heuristic arguments have been supported by rigorous ones by use of an operator inequality due to Bogoliubov.<sup>66,259</sup>

The Bogoliubov inequality can be introduced by the following arguments. Let us consider a scalar product  $(A, B)$  of two operators  $A$  and  $B$  defined in the previous section

$$(A, B) = \frac{1}{Z} \sum_{n \neq m} \langle n|A^\dagger|m\rangle \langle m|B|n\rangle \left( \frac{\exp -(E_m/k_B T) - \exp -(E_n/k_B T)}{E_n - E_m} \right). \tag{10.33}$$

We have obvious inequality

$$(A, B) \leq \frac{1}{2k_B T} \langle AA^\dagger + A^\dagger A \rangle. \tag{10.34}$$

Then we make use of the Cauchy-Schwartz inequality (10.27) which has the form

$$|(A, B)|^2 \leq (A, A)(B, B). \tag{10.35}$$

If we take  $B = [C^\dagger, H]_-$ , we arrive at the Bogoliubov inequality

$$|\langle [C^\dagger, A^\dagger]_- \rangle|^2 \leq \frac{1}{2k_B T} \langle A^\dagger A + AA^\dagger \rangle \langle [C^\dagger, [H, C]_-]_- \rangle. \tag{10.36}$$

In a more formal language, we can formulate this as follows. Let us suppose that  $H$  is a symmetrical operator in the Hilbert space  $L$ . For an operator  $X$  in  $L$ , let us define

$$\langle X \rangle = \frac{1}{Z} \text{Tr } X \exp(-H/k_B T); \quad Z = \text{Tr } \exp(-H/k_B T). \tag{10.37}$$

The Bogoliubov inequality for operators  $A$  and  $C$  in  $L$  has the form

$$\frac{1}{2k_B T} \langle AA^\dagger + A^\dagger A \rangle \langle [[C, H]_-, C^\dagger]_- \rangle \geq |\langle [C, A]_- \rangle|^2. \tag{10.38}$$



The Bogoliubov inequality can be rewritten in a slightly different form

$$k_B T \langle |[C, A]_- \rangle|^2 / \langle [[C, H]_-, C^\dagger]_- \rangle \leq \frac{\langle [A, A^\dagger]_+ \rangle}{2}. \quad (10.39)$$

It is valid for arbitrary operators  $A$  and  $C$ , provided the Hamiltonian is Hermitian and the appropriate thermal averages exist. The operators  $C$  and  $A$  are chosen in such a way that the numerator on the left-hand side reduces to the order parameter and the denominator approaches zero in the limit of a vanishing ordering field. Thus the upper limit placed on the order parameter vanishes when the symmetry-breaking field is reduced to zero.

The very elegant piece of work by Bogoliubov<sup>66</sup> stimulated numerous investigations on the upper and lower bounds for thermodynamic averages.<sup>142,259,263–276</sup> A. B. Harris<sup>263</sup> analyzed the upper and lower bounds for thermodynamic averages of the form  $\langle [A, A^\dagger]_+ \rangle$ . From the lower bound he derived a special case of the Bogoliubov inequality of the form

$$\langle A^\dagger A \rangle \geq \langle [A, A^\dagger]_- \rangle / (\exp(\beta\langle \omega \rangle) - 1) \quad (10.40)$$

and a few additional weaker inequalities.

The rigorous consideration of the Bogoliubov inequality was carried out by Garrison and Wong.<sup>264</sup> They pointed rightly that in the conventional Green's function approach to statistical mechanics all relations are first derived for strictly finite systems; the thermodynamic limit is taken at the end of the calculation. Since the original derivation of the Bogoliubov inequalities was carried out within this framework, the subsequent applications had to follow the same prescription. It was applied by a number of authors to show the impossibility of various kinds of long-range order in one- and two-dimensional systems. In the latter class of problems, a special difficulty arises from the fact that finite systems do not exhibit the broken symmetries usually associated with long-range order. This has led to the use of Bogoliubov's quasiaveraging method in which the finite-system Hamiltonian was modified by the addition of a symmetry breaking term, which was set equal to zero only after the passage to the thermodynamic limit. Authors emphasized that this approach has never been shown to be equivalent to the more rigorous treatment of broken symmetries provided by the theory of integral decompositions of states on  $C^*$ -algebras; furthermore, for some problems (e.g., Bose condensation and anti-ferromagnetism) the symmetry breaking term has no clear physical interpretation. Garrison and Wong<sup>264</sup> show how these difficulties can be avoided by establishing the Bogoliubov inequalities directly in the thermodynamic limit. In their work, the Bogoliubov inequalities were derived for the infinite volume states describing the thermodynamic limits of physical systems. The only property of the states required is that they satisfy the Kubo–Martin–Schwinger boundary condition. Roepstorff<sup>266</sup> investigated a stronger version of Bogoliubov's inequality and the Heisenberg model. He derived a rigorous upper bound for the magnetization in the ferromagnetic quantum Heisenberg model with arbitrary spin and dimension  $D \geq 3$  on the basis of general inequalities in quantum statistical mechanics.

Further generalization was carried out by L. Pitaevskii and S. Stringari<sup>268</sup> who carefully reconsidered the interrelation of the uncertainty principle, quantum fluctuations, and broken symmetries for many-particle interacting systems. At zero temperature, the Bogoliubov inequality provides significant information on the static polarizability, but not directly on the fluctuations occurring in the system. Pitaevskii and Stringari<sup>268</sup> presented a different inequality yielding, at low temperature, relevant information on the fluctuations of physical quantities

$$\int d\omega J(A^\dagger, A; \omega) \coth \frac{\beta\omega}{2} \int d\omega J(B^\dagger, B; \omega) \tanh \frac{\beta\omega}{2} \geq \left| \int d\omega J(A^\dagger, B; \omega) \right|^2. \tag{10.41}$$

They also show that the following inequality holds

$$\langle [A^\dagger, A]_+ \rangle \langle [B^\dagger, B]_+ \rangle \geq |\langle [A^\dagger, B]_- \rangle|^2. \tag{10.42}$$

The inequality (10.41) can be applied to both Hermitian and non-Hermitian operators and can be consequently regarded as a natural generalization of the Heisenberg uncertainty principle. Its determination is based on the use of the Schwartz inequality for auxiliary operators related to the physical operators through a linear transformation. The inequality (10.41) was employed to derive useful constraints on the behavior of quantum fluctuations in problems with continuous group symmetries. Applications to Bose superfluids, antiferromagnets and crystals at zero temperature were discussed as well. In particular, a simple and direct proof of the absence of long range order at zero temperature in the 1D case was formulated. Note that inequality (10.41) does not coincide, except at  $T = 0$ , with inequality (10.42) because of the occurrence of the tanh factor instead of the coth one in the integrand of the left-hand side containing  $J(B^\dagger, B; \omega)$ . However, the inequality (10.42) follows immediately from inequality (10.41) using the inequality<sup>268</sup>

$$J(B^\dagger, B; \omega) \coth \frac{\beta\omega}{2} \geq J(B^\dagger, B; \omega) \tanh \frac{\beta\omega}{2}. \tag{10.43}$$

The Bogoliubov inequality

$$\langle [A^\dagger, A]_+ \rangle \langle [B^\dagger, [H, B]_-]_- \rangle \geq \frac{2}{\beta} |\langle [A^\dagger, B]_- \rangle|^2 \tag{10.44}$$

can be obtained from (10.41) using the inequality (10.43). Pitaevskii and Stringari<sup>268</sup> noted, however, that in general their inequality (10.42) for the fluctuations of the operator  $A$  differs from the Bogoliubov inequality (10.44) in an important way. In fact, result (10.44) provides particularly strong conditions when  $k_B T$  is larger than the typical excitation energies induced by the operator  $A$  and explains in a simple way the divergent  $k_B T/q^2$  behavior exhibited by the momentum distribution of Bose superfluids as well as from the transverse structure factor in antiferromagnets. Vice-versa, inequality (10.42) is useful when  $k_B T$  is smaller than the typical excitation energies and consequently emphasizes the role of the zero

point motion of the elementary excitations which is at the origin of the  $1/q^2$  behavior. The general inequality (10.41) provides in their opinion the proper interpolation between the two different regimes.

Thus Pitaevskii and Stringari proposed a zero-temperature analogue of the Bogoliubov inequality, using the uncertainty relation of quantum mechanics. They presented a method for showing the absence of breakdown of continuous symmetry in the ground state. T. Momoi<sup>277</sup> developed their ideas further. He discussed conditions for the absence of spontaneous breakdown of continuous symmetries in quantum lattice systems at  $T = 0$ . His analysis was based on Pitaevskii and Stringari's idea that the uncertainty relation can be employed to show quantum fluctuations. For one-dimensional systems, it was shown that the ground state is invariant under a continuous transformation if a certain uniform susceptibility is finite. For the two- and three-dimensional systems, it was shown that truncated correlation functions cannot decay any more rapidly than  $|r|^{-d+1}$  whenever the continuous symmetry is spontaneously broken. Both of these phenomena occur owing to quantum fluctuations. The Momoi's results cover a wide class of quantum lattice systems having not-too-long-range interactions.

An important aspect of the later use of Bogoliubov's results was their application to obtain rigorous proofs of the absence of specific ordering in one- and two-dimensional systems of many particles interacting through binary potentials with a definite restriction on the interaction.<sup>37,66,68,259</sup> The problem of the presence or absence of phase transitions in systems with short-range interaction has been discussed for quite a long time. The physical reasons why specific ordering cannot occur in one- and two-dimensional systems is known. The creation of a macroscopic region of disorder with characteristic scale  $\sim L$  requires negligible energy ( $\sim L^{d-2}$  if the interaction has a finite range). However, a unified approach to this problem was lacking and few rigorous results were obtained.<sup>259</sup>

Originally, the Bogoliubov inequality was applied to exclude ordering in isotropic Heisenberg ferromagnets and antiferromagnets by Mermin and Wagner<sup>269</sup> and in one or two dimensions in superconducting and superfluid systems by Hohenberg<sup>270</sup> (see also Refs. 271–276). The physics behind the Mermin-Wagner theorem is based on the conjecture that the excitation of spin waves can destroy the magnetic order since the density of states of the excitations depends on the dimensionality of the system. In  $D = 2$  dimensions, thermal excitations of spin waves destroy long-range order. The number of thermal spin excitations is

$$\mathcal{N} = \sum_k \langle N_k \rangle = \sum_k \frac{1}{\exp(\beta E_k) - 1} \sim \int \frac{k^{D-1} dk}{\exp(\beta D_{\text{sw}} k^2) - 1} \sim \int \frac{k^D dk}{k^3} \quad (10.45)$$

This expression diverges for  $D = 2$ . Thus the ground state is unstable to thermal excitation. The reason for the absence of magnetic order under the above assumptions is that at finite temperatures, spin waves are easily excitable, what destroys magnetic order.

In their paper, exploiting a thermodynamic inequality due to Bogoliubov,<sup>66</sup>

Mermin and Wagner<sup>269</sup> formulated the statement that for one- or two-dimensional Heisenberg systems with isotropic interactions of the form

$$H = \frac{1}{2} \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j - h S_{\vec{q}}^z \tag{10.46}$$

and such that the interactions are short-ranged, namely which satisfy the condition

$$\mathcal{J} = \frac{1}{2N} \sum_{i,j} |J_{ij}| |\vec{r}_i - \vec{r}_j|^2 < \infty, \tag{10.47}$$

cannot be ferro- or antiferromagnetic. Here  $S_{\vec{q}}^z$  is the Fourier component of  $S_i^z$ ,  $N$  is the number of spins. Consider the inequality (10.38) and take  $C = S_{\vec{k}}^z$  and  $A = S_{-\vec{k}-\vec{q}}^y$ . It follows from (10.38) that

$$\frac{\langle S_{\vec{q}}^z \rangle}{N} \leq \frac{1}{\hbar^2 k_B T} S_{yy}(\vec{k} + \vec{q}) \frac{1}{N} \langle [S_{-\vec{k}}^x, [H, S_{\vec{k}}^x]_-]_- \rangle. \tag{10.48}$$

Here  $S_{yy}(\vec{q}) = \langle S_{\vec{q}}^y S_{-\vec{q}}^y \rangle / N$ . The direct calculation leads to the equality

$$\begin{aligned} \Lambda(k) &= \frac{1}{N} \langle [S_{-\vec{k}}^x, [H, S_{\vec{k}}^x]_-]_- \rangle \\ &= \hbar^2 \left( h \frac{\langle S_{\vec{q}}^z \rangle}{N} + \frac{1}{N} \sum_{j,j'} |J_{jj'}| (\cos \vec{k}(\vec{r}_{j'} - \vec{r}_j) - 1) \langle S_j^y S_{j'}^y + S_j^z S_{j'}^z \rangle \right). \end{aligned} \tag{10.49}$$

Thus we have

$$\Lambda(k) \leq \hbar^2 \left( h \frac{\langle S_{\vec{q}}^z \rangle}{N} + S(S+1) \mathcal{J} k^2 \right). \tag{10.50}$$

It follows from the Eqs. (10.48) and (10.50) that

$$S_{yy}(\vec{k} + \vec{q}) \geq \frac{k_B T h \frac{\langle S_{\vec{q}}^z \rangle^2}{N^2}}{h \frac{\langle S_{\vec{q}}^z \rangle}{N} + S(S+1) \mathcal{J} k^2}. \tag{10.51}$$

To proceed, it is necessary to sum up  $(1/N \sum_k)$  on both sides of the inequality (10.51). After doing that we obtain

$$\frac{k_B T \frac{\langle S_{\vec{q}}^z \rangle^2}{N^2}}{(2\pi)^D} \int_0^{\vec{K}} \frac{F_D k^{D-1} dk}{h \frac{\langle S_{\vec{q}}^z \rangle}{N} + S(S+1) \mathcal{J} k^2} \leq S(S+1). \tag{10.52}$$

The following notation was introduced

$$F_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}. \tag{10.53}$$

Here  $\Gamma(D/2)$  is the gamma function. Considering the two-dimensional case we find that

$$h \frac{\langle S_{\vec{q}}^z \rangle}{N} \leq \text{const} \frac{S(S+1)\sqrt{\mathcal{J}}}{\sqrt{T}} \frac{1}{\sqrt{|\ln|\hbar|}}. \tag{10.54}$$

Thus, at any non-zero temperature, a one- or two-dimensional isotropic spin- $S$  Heisenberg model with finite-range exchange interaction cannot be neither ferromagnetic nor antiferromagnetic.

In other words, according to the Mermin–Wagner theorem, there can be no long range order at any non-zero temperature in one- or two-dimensional systems whenever this ordering would correspond to the breaking of a continuous symmetry and the interactions fall off sufficiently rapidly with inter-particle distance.<sup>278</sup> The Mermin–Wagner theorem follows from the fact that in one and two-dimensions a diverging number of infinitesimally low energy excitations is created at any finite temperature and therefore in these cases the assumption of there being a non-vanishing order parameter is not self-consistent. The proof does not apply to  $T = 0$ , thus the ground state itself may be ordered. Two dimensional ferromagnetism is possible strictly at  $T = 0$ . In this case quantum fluctuations oppose, but do not prevent a finite order parameter from appearing in a ferromagnet. In contrast, for one dimensional systems, quantum fluctuations tend to become so strong that they prevent ordering, even in the ground state.<sup>277</sup>

Note that the basic assumptions of the Mermin–Wagner theorem (isotropic and short-range<sup>278,279</sup> interaction) are usually not strictly fulfilled in real systems. Thorpe<sup>280</sup> applied the method of Mermin and Wagner to show that one- and two-dimensional spin systems interacting with a general isotropic interaction

$$H = \frac{1}{2} \sum_{ijn} J_{ij}^{(n)} (\vec{S}_i \cdot \vec{S}_j)^n, \quad (10.55)$$

where the exchange interactions  $J_{ij}^{(n)}$  are of finite range, cannot order in the sense that  $\langle O_i \rangle = 0$  for all traceless operators  $O_i$  defined at a single site  $i$ . Mermin and Wagner have proved the above for the case  $n = 1$  with  $O_i = \vec{S}_i$ , i.e., for the Heisenberg Hamiltonian (10.46). Thorpe's results show that a small isotropic bi-quadratic exchange  $(\vec{S}_i \cdot \vec{S}_j)^2$  cannot induce ferromagnetism or antiferromagnetism in a two-dimensional Heisenberg system. The proof utilizes the Bogoliubov inequality (10.44). Further discussion of the results of Mermin and Wagner and Thorpe was carried out in Ref. 281. The Hubbard identity was used to show the absence of magnetic phase transitions in Heisenberg spin systems in one and two dimensions, generalizing Mermin and Wagner's next term result in an alternative way as Thorpe has done.

The results of Mermin and Wagner and Thorpe show that the isotropy of the Hamiltonian plays the essential role. However it is clear that although one- and two-dimensional systems exist in nature that may be very nearly isotropic, they all have a small amount of anisotropy. Experiments suggested that a small amount of anisotropy can induce a spontaneous magnetization in two dimensions. Froehlich and Lieb<sup>282</sup> proved the existence of phase transitions for anisotropic Heisenberg models. They show rigorously that the two-dimensional anisotropic, nearest-neighbor Heisenberg model on a square lattice, both quantum and classical, have a phase transition in the sense that the spontaneous magnetization is

positive at low temperatures. This is so for all anisotropies. An analogous result (staggered polarization) holds for the antiferromagnet in the classical case; in the quantum case, it holds if the anisotropy is large enough (depending on the single-site spin).

Since then, this method has been applied to show the absence of crystalline order in classical systems,<sup>273–276</sup> the absence of an excitonic insulating state,<sup>283</sup> to rule out long-range spin density waves in an electron gas<sup>284</sup> and magnetic ordering in metals.<sup>285,286</sup> The systems considered include not only one- and two-dimensional lattices, but also three-dimensional systems of finite cross section or thickness.<sup>276</sup>

In this way the inequalities have been applied by Josephson<sup>287</sup> to derive rigorous inequalities for the specific heat in either one- or two-dimensional systems. A rigorous inequality was derived relating the specific heat of a system, the temperature derivative of the expectation value of an arbitrary operator and the mean-square fluctuation of the operator in an equilibrium ensemble. The class of constraints for which the theorem was shown to hold includes most of those of practical interest, in particular the constancy of the volume, the pressure, and (where applicable) the magnetization and the applied magnetic field.

Ritchie and Mavroyannis<sup>288</sup> investigated the ordering in systems with quadrupolar interactions and proved the absence of ordering in quadrupolar systems of restricted dimensionality. The Bogoliubov inequality was applied to the isotropic model to show that there is no ordering in one- or two-dimensional systems. Some properties of the anisotropic model were presented. Thus in this paper it was shown that an isotropic quadrupolar model does not have macroscopic order in one or two dimensions.

The statements above on the impossibility of magnetic order or other long-range order in one and two spatial dimensions can be generalized to other symmetry broken states and to other geometries, such as fractal systems,<sup>289–291</sup> Heisenberg<sup>292</sup> thin films, etc. In Ref. 292, thin films were described as idealized systems having finite extent in one direction but infinite extent in the other two. For systems of particles interacting through smooth potentials (e.g., no hard cores), it was shown<sup>292</sup> that an equilibrium state for a homogeneous thin film is necessarily invariant under any continuous internal symmetry group generated by a conserved density. For short-range interactions it was also shown that equilibrium states are necessarily translation invariant. The absence of long-range order follows from its relation to broken symmetry. The only properties of the state required for the proof are local normality, spatial translation invariance, and the Kubo–Martin–Schwinger boundary condition. The argument employs the Bogoliubov inequality and the techniques of the algebraic approach to statistical mechanics. For inhomogeneous systems, the same argument shows that all order parameters defined by anomalous averages must vanish. Identical results can be obtained for systems with infinite extent in one direction only.

In the case of thin films the Mermin–Wagner theorem provides an important leading idea and gives a qualitative explanation<sup>293</sup> why the ordering temperature

$T_c$  is usually reduced for thinner films. Two models of magnetic bilayers were considered in Ref. 294, both based on the Heisenberg model. In the first case of ferromagnetically ordered ferromagnetically coupled planes of  $S = 1$ , the anisotropy is of easy plane/axis type, while in the study of antiferromagnetically ordered antiferromagnetically coupled planes of  $S = 1/2$ , the anisotropy is of  $XXZ$  type. Both systems were treated by Green's function method, which consistently applied within random phase approximation. The calculations lead to excitation energies and the system of equations for order parameters which can be solved numerically and which satisfies both Mermin–Wagner and Goldstone theorem in the corresponding limit and also agrees with the mean field results. The basic result was that the transition temperature for magnetic dipole order parameter is unique for both planes. Nonexistence of magnetic order in the Hubbard model of thin films was shown in Ref. 295. Introduction of the Stoner molecular field approximation is responsible for the appearance of magnetic order in the Hubbard model of thin films.

The Mermin–Wagner theorem was strengthened by Bruno<sup>296</sup> so as to rule out magnetic long-range order at  $T > 0$  in one- or two-dimensional Heisenberg and  $XY$  systems with long-range interactions decreasing as  $R^{-\alpha}$  with a sufficiently large exponent  $\alpha$ . For oscillatory interactions, ferromagnetic long-range order at  $T > 0$  is ruled out if  $\alpha \geq 1$  ( $D = 1$ ) or  $\alpha > 5/2$  ( $D = 2$ ). For systems with monotonically decreasing interactions, ferro- or antiferromagnetic long-range order at  $T > 0$  is ruled out if  $\alpha \geq 2D$ . In view of the fact that most magnetic ultrathin films investigated experimentally consist of metals and alloys, these results are of great importance.

The Mermin–Wagner theorem states that at non-zero temperatures, the two dimensional Heisenberg model has no spontaneous magnetization. A global rotation of spins in a plane means that we cannot have a long-range magnetic ordering at non-zero temperature. Consequently the spin-spin correlation function decays to zero at large distances, although the Mermin–Wagner theorem gives no indication of the rate of decay. Martin<sup>297</sup> shows that the Goldstone theorem in any dimension and the absence of symmetry breaking in two dimensions result from a simple use of the Bogoliubov inequality. Goldstone theorem is the statement that an equilibrium phase which breaks spontaneously a continuous symmetry must have a slow (non-exponential) clustering. The classical arguments about the absence of symmetry breakdown in two dimensions were formulated in a few earlier studies, where it was proved that in any dimension, a phase of a lattice system which breaks a continuous internal symmetry cannot have an integrable clustering. Classical continuous systems were also studied in all dimensions with the result that the occurrence of crystalline or orientational order implies a slow clustering. The same property holds for Coulomb systems. In particular, the rate of clustering of particle correlation functions in a 3-dimensional classical crystal is necessarily slower or equal to  $|x|^{-1}$  (see also Refs. 298–300).

Landau, Peres, and Wreszinski<sup>267</sup> proved a Goldstone-type theorem for a wide class of lattice and continuum quantum systems, both for the ground state and at

nonzero temperature. For the ground state ( $T = 0$ ) spontaneous breakdown of a continuous symmetry implies no energy gap. For nonzero temperature, spontaneous symmetry breakdown implies slow clustering (no  $L^1$  clustering). The methods applied also to nonzero-temperature classical systems. They showed that for a physical system with short-range forces and a continuous symmetry, if the ground state is not invariant under the symmetry, the Goldstone theorem states that the system possesses excitations of arbitrarily low energy. In the case of the ground state (vacuum) of local quantum field theory, the existence of an energy gap is equivalent to exponential clustering. For general ground states of non-relativistic systems, the two properties (energy gap and clustering) are, however, independent and, in particular, the assumption that the ground state is the unique vector invariant under time translations does not necessarily follow from the assumption of spacelike clustering. Another related aspect, of greater relevance to their discussion, is the fact that the rate of clustering is not expected to be related to symmetry breakdown and absence of an energy gap, since for example the ground state of the Heisenberg ferromagnet has a broken symmetry and no energy gap, but is exponentially clustering (for the ground state is a product state of spins pointing in a fixed direction). On the other hand, for  $T > 0$ , no energy gap is expected to occur, at least under general timelike clustering assumptions. These assumptions may be verified for the free Bose gas. At nonzero temperature, it is the cluster properties that are important in connection with symmetry breakdown. At nonzero temperature, the authors formulated the Goldstone theorem as follows. Given a system with short-range forces and a continuous symmetry, if the equilibrium state is not invariant under the symmetry, then the system does not possess exponential clustering.

Landau, Peres, and Wreszinski<sup>267</sup> explored the validity of the Goldstone theorem for a wide class of spin systems and many-body systems, both for the ground state and at nonzero temperature. The main tool that was used at nonzero temperature was the Bogoliubov inequality, which is valid for both classical and quantum systems. Their results apply to states which are invariant with respect to spatial translations by some discrete set which is sufficiently dense. (For lattice systems this could be a sublattice, and for continuum systems, a lattice imbedded in the continuum.) They proved that for interactions which are not too long range, for the ground state ( $T = 0$ ) spontaneous breakdown of a continuous symmetry implies no energy gap. For nonzero temperature ( $T > 0$ ) spontaneous symmetry breakdown implies no exponential clustering (in fact no  $L^1$  clustering).

Rastelli and Tassi<sup>301</sup> pointed that the theorem of Mermin and Wagner excludes long-range order in one- and two-dimensional Heisenberg models at any finite temperature if the exchange interaction is short ranged. In their opinion, strong but nonrigorous indications exist about the absence of long-range order even in three-dimensional Heisenberg models when suitable competing exchange interactions are present. They argued, as a rigorous consequence of the Bogoliubov inequality, that this expectation may be true. It was found that for models where the exchange



competition concerns at least two over three dimensions, a surface of the parameter space exists where long-range order is absent. This surface meets at vanishing temperature the continuous phase-transition line which is the border line between the ferromagnetic and helical configuration. They also investigated the spherical model<sup>302</sup> and concluded that the spherical model is a unique model for which an exact solution at finite temperature exists in three dimensions. In that paper they proved that this model may show an absence of long-range order in three dimensions if a suitable competition between exchange couplings was assumed. In particular they found an absence of long-range order in wedge-shaped regions around the ferromagnet- or antiferromagnet-helix transition line or in the vicinity of a degeneration line, where infinite nonequivalent isoenergetic helix configurations are possible. They evaluated explicitly the phase diagram of a tetragonal antiferromagnet with exchange couplings up to third neighbors but their conclusions apply as well to any Bravais lattice.

The problem of generalization of the Mermin–Wagner theorem for the Heisenberg spin-glass order was discussed in Refs. 303–305. Using the Bogoliubov inequality, Fernandez<sup>305</sup> considered the isotropic Heisenberg Hamiltonian

$$H = - \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \vec{S}_j, \quad (10.56)$$

which was used to model spin-glass behavior. The purpose of the model being to produce  $|\langle S_i^z \rangle| \neq 0$  below a certain temperature without the presence of long-range spatial order. Fernandez showed that there can be no spin-glass in one or two dimensions for isotropic Heisenberg Hamiltonians for  $T \neq 0$  if

$$\lim_{N \rightarrow \infty} N^{-1} \sum_{\langle ij \rangle} |J_{ij}| (\vec{r}_i - \vec{r}_j)^2 < \infty. \quad (10.57)$$

In summary, the Mermin–Wagner theorem, which excludes the breaking of a continuous symmetry in two dimensions at finite temperatures, was established in 1966. Since then, various more precise and more general versions have been considered (see Refs. 300, 306–311). These considerations of symmetry broken systems are important in order to establish whether or not long-range order is possible in various concrete situations.

The fact that the zero magnetism which is enforced by the Mermin–Wagner theorem is compatible with various types of phase transitions was noted by many authors. For example, Dyson, Lieb and Simon<sup>312,313</sup> proved the existence of a phase transition at non-zero temperature for the Heisenberg model with nearest neighbor coupling. The proof essentially relied on some new inequalities involving two-point functions. Some of these inequalities are quite general and, therefore, apply to any quantum system in thermal equilibrium. Others rest on the specific structure of the model (spin system, simple cubic lattice, nearest neighbor coupling, etc.) and have limited applicability.

The low dimensional systems show large fluctuations for continuous symmetry.<sup>300</sup> The Hohenberg–Mermin–Wagner theorem states that the corresponding

spontaneous magnetizations are vanishing at finite temperatures in one and two dimensions. Since their articles appeared, their method has been applied to various systems, including classical and quantum magnets, interacting electrons in a metal and Bose gas. The theorem was extended to the models on a class of generic lattices with the fractal dimension by Cassi.<sup>289–291</sup> In a stronger sense, it was also proved for a class of low-dimensional systems that the equilibrium states are invariant under the action of the continuous symmetry group. Even at zero temperature, the same is true if the corresponding one- or two-dimensional system satisfies conditions such as boundedness of susceptibilities. Since a single spin shows the spontaneous magnetization at zero temperature, the absence of the spontaneous symmetry breaking implies that the strong fluctuations due to the interaction destroy the ordering and lead to the finite susceptibilities. In other words, one cannot expect the absence of spontaneous symmetry breaking at zero temperature in a generic situation.<sup>300</sup>

Some other applications of the Bogoliubov inequality to various problems of statistical physics were discussed in Refs. 314–319.

## 11. Broken Symmetries and Condensed Matter Physics

Studies of symmetries and the consequences of breaking them have led to deeper understanding in many areas of science. Condensed matter physics is the field of physics that deals with the macroscopic physical properties of matter. In particular, it is concerned with the *condensed* phases that appear whenever the number of constituents in a system is extremely large and the interactions between the constituents are strong. The most familiar examples of condensed phases are solids and liquids, which arise from the electric force between atoms. More exotic condensed phases include the superfluid and the Bose–Einstein condensate found in certain atomic systems.<sup>320–323</sup> Symmetry has always played an important role in condensed matter physics,<sup>323</sup> from fundamental formulations of basic principles to concrete applications.<sup>239,242,243,324–332</sup> In condensed matter physics, the symmetry is important in classifying different phases and understanding the phase transitions between them. The phase transition is a physical phenomenon that occurs in macroscopic systems and consists of the following. In certain equilibrium states of the system, an arbitrary small influence leads to a sudden change of its properties: the system passes from one homogeneous phase to another. Mathematically, a phase transition is treated as a sudden change of the structure and properties of the Gibbs distributions describing the equilibrium states of the system, for arbitrary small changes of the parameters determining the equilibrium.<sup>333</sup> The crucial concept here is the order parameter.

In statistical physics, the question of interest is to understand how the order of phase transition in a system of many identical interacting subsystems depends on the degeneracies of the states of each subsystem and on the interaction between subsystems. In particular, it is important to investigate the role of the symmetry

and uniformity of the degeneracy and the symmetry of the interaction. Statistical mechanical theories of the system composed of many interacting identical subsystems have been developed frequently for the case of ferro- or antiferromagnetic spin system, in which the phase transition is usually found to be one of second order unless it is accompanied with such an additional effect as spin-phonon interaction. The phase transition of first order also occurs in a variety of systems, such as ferroelectric transition, orientational transition and so on. Second order phase transitions are frequently, if not always, associated with spontaneous breakdown of a global symmetry. It is then possible to find a corresponding order parameter which vanishes in the disordered phase and is nonzero in the ordered phase. Qualitatively the transition is understood as condensation of the broken symmetry *charge* carriers. The critical region is effectively described by a local Lagrangian involving the order parameter field.<sup>27</sup>

Combining many elementary particles into a single interacting system may result in collective behavior that qualitatively differs from the properties allowed by the physical theory governing the individual building blocks as was stressed by Anderson.<sup>94</sup> It is known that the description of spontaneous symmetry breaking that underlies the connection between classically ordered objects in the thermodynamic limit and their individual quantum-mechanical building blocks is one of the cornerstones of modern condensed-matter theory and has found applications in many different areas of physics. The theory of spontaneous symmetry breaking, however, is inherently an equilibrium theory, which does not address the dynamics of quantum systems in the thermodynamic limit. J. van Wezel<sup>334</sup> investigated the quantum dynamics of many particle system in the thermodynamic limit. Author used the example of a particular antiferromagnetic model system to show that the presence of a so-called thin spectrum of collective excitations with vanishing energy — one of the well-known characteristic properties shared by all symmetry breaking objects — can allow these objects to also spontaneously break time-translation symmetry in the thermodynamic limit. As a result, that limit is found to be able, not only to reduce quantum-mechanical equilibrium averages to their classical counterparts, but also to turn individual-state quantum dynamics into classical physics. In the process, van Wezel found that the dynamical description of spontaneous symmetry breaking can also be used to shed some light on the possible origins of Born's rule. The work was concluded by describing an experiment on a condensate of exciton polaritons which could potentially be used to experimentally test the proposed mechanism.

There is an important distinction between the case where the broken symmetry is continuous (e.g., translation, rotation, gauge invariance) or discrete (e.g., inversion, time reversal symmetry). The Goldstone theorem states that when a continuous symmetry is spontaneously broken and the interactions are short ranged, a collective mode (excitation) exists with a gapless energy spectrum (i.e., the energy dispersion curve starts at zero energy and is continuous). Acoustical phonons in a crystal are prime examples of such so-called gapless Goldstone modes. Other exam-

ples are the Bogoliubov sound modes in (charge neutral) Bose condensates<sup>320,322</sup> and spin waves (magnons) in ferro- and antiferromagnets. On the same ground, one can consider the existence of magnons in spin systems at low temperatures,<sup>335</sup> acoustic and optical vibration modes in regular lattices or in multi-sublattice magnets, as well as the vibration spectra of interacting electron and nuclear spins in magnetically-ordered crystals.<sup>328</sup>

It was claimed by some authors that there exists a certain class of systems with broken symmetry, whose condensed state and ensuring macroscopic theory are quite analogous to those of superfluid helium. These systems are Heisenberg magnetic lattices, both ferro- and antiferromagnetic, for which the macroscopic modes associated with the *quasi-conservation law* are long-wavelength spin waves. In contrast to liquid helium, those systems are amenable to a fully microscopic analysis, at least in the low-temperature limit. However, there are also differences in the nature of antiferromagnetism and superconductivity for many-particle systems on a lattice. It is therefore of interest to look carefully into the specific features of the magnetic, superconducting and Bose systems in some detail, both for its own sake, and to gain insight into the general principles of their behavior.

### 11.1. *Superconductivity*

The BCS-Bogoliubov model of superconductivity is one of few examples in the many particle system that can be solved (asymptotically) exactly.<sup>37,97,98,336–341</sup> In the limit of infinite volume, the BCS-Bogoliubov theory of superconductivity provides an exactly soluble model<sup>37,97,98,336</sup> wherein the phenomenon of spontaneous symmetry breakdown occurs explicitly. The symmetry that gets broken being the gauge invariance.

It was shown in previous sections that the concept of spontaneously broken symmetry is one of the most important notions in statistical physics, in the quantum field theory and elementary particle physics. This is especially so as far as creating a unified field theory, uniting all the different forces of nature,<sup>31,51,112,342</sup> is concerned. One should stress that the notion of spontaneously broken symmetry came to the quantum field theory from solid-state physics.<sup>47</sup> It was originated in quantum theory of magnetism,<sup>102,103</sup> and later was substantially developed and found wide applications in the gauge theory of elementary particle physics.<sup>51,54,93</sup> It was in the quantum field theory where the ideas related to that concept were quite substantially developed and generalized. The analogy between the Higgs mechanism giving mass to elementary particles and the Meissner effect in the Ginzburg–Landau superconductivity theory is well-known.<sup>47,100,101,144–146</sup>

The Ginzburg–Landau model is a special form of the mean-field theory.<sup>242,243</sup> The superconducting state has lower entropy than the normal state and is therefore the more ordered state. A general theory based on just a few reasonable assumptions about the order parameter is remarkably powerful.<sup>242,243</sup> It describes not just BCS-Bogoliubov superconductors but also the high- $T_c$  superconductors, superfluids, and

Bose–Einstein condensates. The Ginzburg–Landau model operates with a pseudo-wave function  $\Psi(\vec{r})$ , which plays the role of a parameter of complex order, while the square of this function modulus  $|\Psi(\vec{r})|^2$  should describe the local density of superconducting electrons. It was conjectured that  $\Psi(\vec{r})$  behaves in many respects like a macroscopic wavefunction but without certain properties associated with linearity: superposition and normalization. It is well-known, that the Ginzburg–Landau theory is applicable if the temperature of the system is sufficiently close to its critical value  $T_c$ , and if the spatial variations of the functions  $\Psi$  and of the vector potential  $\vec{A}$  are not too large. The main assumption of the Ginzburg–Landau approach is the possibility to expand the free-energy density  $f$  in a series under the condition, that the values of  $\Psi$  are small, and its spatial variations are sufficiently slow. The Ginzburg–Landau equations follow from an application of the variational method to the proposed expansion of the free energy density in powers of  $|\Psi|^2$  and  $|\nabla\Psi|^2$ , which leads to a pair of coupled differential equations for  $\Psi(\vec{r})$  and the vector potential  $\vec{A}$ . The Lawrence–Doniach model was formulated in the paper<sup>343</sup> for analysis of the role played by layered structures in superconducting materials.<sup>344–346</sup> The model considers a stack of two parallel dimensional superconducting layers separated by an isolated material (or vacuum), with a nonlinear interaction between the layers. It was also assumed that an external magnetic field is applied to the system. In some sense, the Lawrence–Doniach model can be considered as an anisotropic version of the Ginzburg–Landau model. More specifically, an anisotropic Ginzburg–Landau model can be considered as a continuous limit approximation to the Lawrence–Doniach model. However, when the coherence length in the direction perpendicular to the layers is less than the distance between the layers, these models are difficult to compare.

Both effects, Meissner effect and Higgs effect are consequences of spontaneously broken symmetry in a system containing two interacting subsystems. According to F. Wilczek,<sup>71</sup> “the most fundamental phenomenon of superconductivity is the Meissner effect, according to which magnetic fields are expelled from the bulk of a superconductor. The Meissner effect implies the possibility of persistent currents. Indeed, if a superconducting sample is subjected to an external magnetic field, currents of this sort must arise near the surface of a sample to generate a cancelling field. An unusual but valid way of speaking about the phenomenon of superconductivity is to say that within a superconductor, the photon acquires a mass. The Meissner effect follows from this.” This is a mechanism by which gauge fields acquire mass: “the gauge particle “eats” a Goldstone boson and thereby becomes massive”. This general idea has been applied to the more complex problem of the weak interaction which is mediated by the  $W$ -bosons. Essentially, the initially massless  $W$ -gauge particles become massive below a symmetry breaking phase transition through a generalized form of the Anderson–Higgs mechanism. This symmetry breaking transition is analogous in some sense to superconductivity with a high transition temperature.

A similar situation is encountered in the quantum solid-state theory.<sup>47</sup> Analogies between the elementary particle and the solid-state theories have both cognitive and practical importance for their development.<sup>47,101,347</sup> We have already discussed the analogies with the Higgs effect playing an important role in these theories. However, we have every reason to also consider analogies with the Meissner effect in the Ginzburg–Landau superconductivity model,<sup>348–351</sup> because the Higgs model is, in fact, only a relativistic analogue of that model.

Gauge symmetry breaking in superconductivity was investigated by W. Kolley.<sup>352,353</sup> The breakdown of the  $U(1)$  gauge invariance in conventional superconductivity was thoroughly reexamined by drawing parallels between the BCS–Bogoliubov and Abelian–Higgs models. The global and local  $U(1)$  symmetries were broken spontaneously and explicitly in view of the Goldstone and Elitzur theorems, respectively. The approximations at which spontaneity comes into the symmetry-breaking condensation, that are differently interpreted in the literature, were clarified. A relativistic version of the Lawrence–Doniach model<sup>218,343,344</sup> was formulated to break the local  $U(1)$  gauge symmetry in analogy to the Anderson–Higgs mechanism. Thereby the global  $U(1)$  invariance is spontaneously broken via the superconducting condensate. The resulting differential-difference equations for the order parameter, the in-plane and inter-plane components of the vector potential are of the Klein–Gordon, Proca and sine-Gordon type, respectively. A comparison with the standard sine-Gordon equation for the superconducting phase difference was given in the London limit. The presented dynamical scheme is applicable to high- $T_c$  cuprates with one layer per unit cell and weak interlayer Josephson tunnelling. The role of the layered structure for the superconducting and normal properties of the correlated metallic systems is the subject of intense discussions<sup>344,345</sup> and studies. N. N. Bogoliubov and then Y. Nambu in their works show that the general features of superconductivity are in fact model independent consequences of the spontaneous breakdown of electromagnetic gauge invariance. S. Weinberg wrote an interesting essay<sup>145</sup> on superconductivity, whose inspiration comes from experience with broken symmetries in particle theory, which was formulated by Nambu. He emphasized that the high-precision predictions about superconductors actually follow not only from the microscopic models themselves, but more generally from the fact that these models exhibit a spontaneous breakdown, electromagnetic gauge invariance in a superconductor. The importance of broken symmetry in superconductivity has been especially emphasized by Anderson.<sup>100,143</sup> One needs detailed models like that BCS–Bogoliubov to explain the mechanism for the spontaneous symmetry breakdown, and as a basis for approximate quantitative calculations, but not to derive the most important exact consequences of this breakdown. To demonstrate this, let us assume that, for whatever reason, electromagnetic gauge invariance in a superconductor was broken. The specific mechanism by which the symmetry breakdown occurs will not be specified for the moment. For this case the electromagnetic gauge group is  $U(1)$ , the group of multiplication of fields  $\psi(x)$  of

charge  $q$  with the phases

$$\psi(x) \rightarrow e^{iq\Lambda/\hbar}\psi(x). \quad (11.1)$$

It is possible to assume that all charges  $q$  are integer multiples of the electron charge  $-e$ , so phases  $\Lambda$  and  $\Lambda + 2\pi\hbar/e$  are to be regarded as identical.<sup>145</sup> This  $U(1)$  is spontaneously broken to  $Z_2$ , the subgroup consisting of  $U(1)$  transformations with  $\Lambda = 0$  and  $\Lambda = \pi\hbar/e$ . The assumption that  $Z_2$  is unbroken arises from the physical picture that, while pairs of electron operators can have non-vanishing expectation value, individual electron operators do not.

In terms of the BCS-Bogoliubov theory of superconductivity<sup>37</sup> this means that the averages  $\langle a_{k\sigma}a_{k-\sigma} \rangle$  and  $\langle a_{k-\sigma}^\dagger a_{k\sigma}^\dagger \rangle$  will be of non-zero value. It is important to emphasize that the BCS-Bogoliubov theory of superconductivity<sup>37,336</sup> was formulated on the basis of a trial Hamiltonian which consists of a quadratic form of creation and annihilation operators, including “anomalous” (off-diagonal) averages.<sup>37</sup> The strong-coupling BCS-Bogoliubov theory of superconductivity was formulated for the Hubbard model in the localized Wannier representation in Refs. 207, 218, 354. Therefore, instead of the algebra of the normal state's operator  $a_{i\sigma}, a_{i\sigma}^\dagger$  and  $n_{i\sigma}$ , for description of superconducting states, one has to use a more general algebra, which includes the operators  $a_{i\sigma}, a_{i\sigma}^\dagger, n_{i\sigma}$  and  $a_{i\sigma}a_{i-\sigma}, a_{i\sigma}^\dagger a_{i-\sigma}^\dagger$ . The relevant generalized one-electron Green function will have the following form:<sup>207,218,354</sup>

$$G_{ij}(\omega) = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} = \begin{pmatrix} \langle\langle a_{i\sigma} | a_{j\sigma}^\dagger \rangle\rangle & \langle\langle a_{i\sigma} | a_{j-\sigma} \rangle\rangle \\ \langle\langle a_{i-\sigma}^\dagger | a_{j\sigma}^\dagger \rangle\rangle & \langle\langle a_{i-\sigma}^\dagger | a_{j-\sigma} \rangle\rangle \end{pmatrix} \quad (11.2)$$

As it was discussed in Refs. 207 and 218, the off-diagonal (anomalous) entries of the above matrix select the vacuum state of the system in the BCS-Bogoliubov form, and they are responsible for the presence of anomalous averages. For treating the problem, we follow the general scheme of the irreducible Green functions method.<sup>207,218</sup> In this approach, we start from the equation of motion for the Green function  $G_{ij}(\omega)$  (normal and anomalous components)

$$\begin{aligned} & \sum_j (\omega\delta_{ij} - t_{ij}) \langle\langle a_{j\sigma} | a_{i'\sigma}^\dagger \rangle\rangle \\ & = \delta_{ii'} + U \langle\langle a_{i\sigma} n_{i-\sigma} | a_{i'\sigma}^\dagger \rangle\rangle + \sum_{nj} V_{ijn} \langle\langle a_{j\sigma} u_n | a_{i'\sigma}^\dagger \rangle\rangle, \end{aligned} \quad (11.3)$$

$$\begin{aligned} & \sum_j (\omega\delta_{ij} + t_{ij}) \langle\langle a_{j-\sigma}^\dagger | a_{i'\sigma}^\dagger \rangle\rangle \\ & = -U \langle\langle a_{i-\sigma}^\dagger n_{i\sigma} | a_{i'\sigma}^\dagger \rangle\rangle + \sum_{nj} V_{jin} \langle\langle a_{j-\sigma}^\dagger u_n | a_{i'\sigma}^\dagger \rangle\rangle. \end{aligned} \quad (11.4)$$

The irreducible Green functions are introduced by definition

$$\begin{aligned}
 {}^{(ir)}\langle\langle a_{i\sigma} a_{i-\sigma}^\dagger | a_{i'\sigma}^\dagger \rangle\rangle_\omega &= \langle\langle a_{i\sigma} a_{i-\sigma}^\dagger | a_{i'\sigma}^\dagger \rangle\rangle_\omega \\
 &\quad - \langle n_{i-\sigma} \rangle G_{11} + \langle a_{i\sigma} a_{i-\sigma} \rangle \langle\langle a_{i-\sigma}^\dagger | a_{i'\sigma}^\dagger \rangle\rangle_\omega, \\
 {}^{(ir)}\langle\langle a_{i\sigma}^\dagger a_{i\sigma} a_{i-\sigma}^\dagger | a_{i'\sigma}^\dagger \rangle\rangle_\omega &= \langle\langle a_{i\sigma}^\dagger a_{i\sigma} a_{i-\sigma}^\dagger | a_{i'\sigma}^\dagger \rangle\rangle_\omega \\
 &\quad - \langle n_{i\sigma} \rangle G_{21} + \langle a_{i\sigma}^\dagger a_{i-\sigma}^\dagger \rangle \langle\langle a_{i\sigma} | a_{i'\sigma}^\dagger \rangle\rangle_\omega.
 \end{aligned} \tag{11.5}$$

The self-consistent system of superconductivity equations follows from the Dyson equation<sup>207,218</sup>

$$\hat{G}_{ii'}(\omega) = \hat{G}_{ii'}^0(\omega) + \sum_{jj'} \hat{G}_{ij}^0(\omega) \hat{M}_{jj'}(\omega) \hat{G}_{j'i'}(\omega). \tag{11.6}$$

The mass operator  $M_{jj'}(\omega)$  describes the processes of inelastic electron scattering on lattice vibrations. The elastic processes are described by the quantity

$$\Sigma_\sigma^c = U \begin{pmatrix} \langle a_{i-\sigma}^\dagger a_{i-\sigma} \rangle & -\langle a_{i\sigma} a_{i-\sigma} \rangle \\ -\langle a_{i-\sigma}^\dagger a_{i\sigma}^\dagger \rangle & -\langle a_{i\sigma}^\dagger a_{i\sigma} \rangle \end{pmatrix}. \tag{11.7}$$

Thus the ‘‘anomalous’’ off-diagonal terms fix the relevant BCS-Bogoliubov vacuum and select the appropriate set of solutions. The functional of the generalized mean field for the superconducting single-band Hubbard model is of the form  $\Sigma_\sigma^c$ . Bogoliubov and Moskalenko<sup>355</sup> have developed an alternative approach to treat the problem of superconductivity for one-band Hubbard model within a diagrammatic technique.

A remark about the BCS-Bogoliubov mean-field approach is instructive. Speaking in physical terms, this theory involves a condensation correctly, in spite that such a condensation cannot be obtained by an expansion in the effective interaction between electrons. Other mean field theories, e.g., the Weiss molecular field theory<sup>333</sup> and the van der Waals theory of the liquid-gas transition are much less reliable. The reason why a mean-field theory of the superconductivity in the BCS-Bogoliubov form is successful would appear to be that the main correlations in metal are governed by the extreme degeneracy of the electron gas. The correlations due to the pair condensation, although they have dramatic effects, are weak (at least in the ordinary superconductors) in comparison with the typical electron energies, and may be treated in an average way with a reasonable accuracy. All the above remarks have relevance to ordinary low-temperature superconductors. In high- $T_c$  superconductors, the corresponding degeneracy temperature is much lower, and the transition temperatures are much higher. In addition, the relevant interaction responsible for the pairing and its strength are unknown yet. From this point of view, the high- $T_c$  systems are more complicated.<sup>356-358</sup> It should be clarified what governs the scale of temperatures, i.e., critical temperature, degeneracy temperature, interaction strength or their complex combination, etc. In this way a useful insight into this extremely complicated problem would be gained. It should be emphasized that the high-temperature superconductors, discovered two decades ago,



motivated an intensification of research in superconductivity, not only because applications are promising, but because they also represent a new state of matter that breaks certain fundamental symmetries.<sup>359–363</sup> These are the broken symmetries of gauge (superconductivity), reflection (*d*-wave superconducting order parameter), and time-reversal (ferromagnetism). Note that general discussion of decay of superconducting and magnetic correlations in one- and two-dimensional Hubbard model was carried out in Ref. 364.

Studies of the high-temperature superconductors confirmed and clarified many important fundamental aspects of superconductivity theory. Kadowaki, Kakeya and Kindo<sup>365</sup> reported about observation of the Nambu–Goldstone mode in the layered high-temperature superconductor  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ . The Josephson plasma resonance (for review see Ref. 366) has been observed in a microwave frequency at 35 GHz in magnetic fields up to 6 T. Making use of the different dispersion relations between two Josephson plasma modes predicted by the recent theories, the longitudinal mode, which is the Nambu–Goldstone mode in a superconductor, was separated out from the transverse one experimentally. This experimental result directly proves the existence of the Nambu–Goldstone mode in a superconductor with a finite energy gap  $\hbar\omega_p = \hbar c/\lambda_c\sqrt{\epsilon}$ . Such a finite energy gap implies the mass of the Nambu–Goldstone bosons in a superconductor, supporting the mass formation mechanism proposed by Anderson.<sup>100,143,144</sup>

Matsui and co-authors<sup>367</sup> performed high-resolution angle-resolved photoemission spectroscopy on triple-layered high- $T_c$  cuprate  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+\delta}$ . They have observed the full energy dispersion (electron and hole branches) of Bogoliubov quasiparticles and determined the coherence factors above and below  $E_F$  as a function of momentum from the spectral intensity as well as from the energy dispersion based on BCS-Bogoliubov theory. The good quantitative agreement between the experiment and the theoretical prediction suggests the basic validity of BCS-Bogoliubov formalism in describing the superconducting state of cuprates.

J. van Wezel and J. van den Brink<sup>368</sup> studied spontaneous symmetry breaking and decoherence in superconductors. They show that superconductors have a thin spectrum associated with spontaneous symmetry breaking similar to that of antiferromagnets, while still being in full agreement with Elitzur's theorem, which forbids the spontaneous breaking of local (gauge) symmetries. This thin spectrum in the superconductors consists of in-gap states that are associated with the spontaneous breaking of a global phase symmetry. In qubits based on mesoscopic superconducting devices, the presence of the thin spectrum implies a maximum coherence time which is proportional to the number of Cooper pairs in the device. Authors presented the detailed calculations leading up to these results and discussed the relation between spontaneous symmetry breaking in superconductors and the Meissner effect, the Anderson–Higgs mechanism, and the Josephson effect. Whereas for the Meissner effect a symmetry breaking of the phase of the superconductor is not required, it is essential for the Josephson effect.

It is of interest to note that the authors of the recent review on the high-temperature superconductivity<sup>369</sup> pointed out that one of the keys to the high-temperature superconductivity puzzle is the *identification of the energy scales* associated with the emergence of a coherent condensate of superconducting electron pairs. These might provide a measure of the pairing strength and of the coherence of the superfluid, and ultimately reveal the nature of the elusive pairing mechanism in the superconducting cuprates. To this end, a great deal of effort has been devoted to investigating the connection between the superconducting transition temperature  $T_c$  and the normal-state pseudogap crossover temperature  $T^*$ . Authors analyzed a large body of experimental data which suggests a coexisting two-gap scenario, i.e., superconducting gap and pseudogap, over the whole superconducting dome. They focused on spectroscopic data from cuprate systems characterized by  $T_c^{\max} \sim 95$  K, such as  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ ,  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ ,  $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$  and  $\text{HgBa}_2\text{CuO}_{4+\delta}$ , with particular emphasis on the Bi-compound which has been the most extensively studied with single-particle spectroscopies. Their analysis have something in common with the concept of the quantum protectorate which emphasizes the importance of the hierarchy of the energy scales.

### 11.2. *Antiferromagnetism*

Superconductivity and antiferromagnetism are both the spontaneously broken symmetries.<sup>240</sup> The idea of antiferromagnetism was first introduced by L. Neel in order to explain the temperature-independent paramagnetic susceptibility of metals like Mn and Cr. According to his idea, these materials consisted of two compensating sublattices undergoing negative exchange interactions. There are two complementary physical pictures of the antiferromagnetic ordering, operated with localized spins and itinerant electrons.<sup>218</sup> L. Neel also formulated the concept of local mean fields.<sup>218</sup> He assumed that the sign of the mean-field could be both positive and negative. Moreover, he showed that below some critical temperature (the Neel temperature) the energetically most favorable arrangement of atomic magnetic moments is such, that there is an equal number of magnetic moments aligned against each other. This novel magnetic structure became known as the antiferromagnetism.<sup>370</sup> It was established that the antiferromagnetic interaction tends to align neighboring spins against each other. In the one-dimensional case, this corresponds to an alternating structure, where an “up” spin is followed by a “down” spin, and vice versa. Later it was conjectured that the state made up from two sublattices inserted into each other is the ground state of the system (in the classical sense of this term). Moreover, the mean-field sign there alternates in the “chessboard” (staggered) order. The question of the true antiferromagnetic ground state is not completely clarified up to the present time. This is related to the fact that, in contrast to ferromagnets, which have a unique ground state, antiferromagnets can have several different optimal states with the lowest energy. The Neel ground state is understood as a possible form of the system’s wave function, describing the antiferromagnetic

ordering of all spins. Strictly speaking, the ground state is the thermodynamically equilibrium state of the system at zero temperature. Whether the Neel state is the ground state in this strict sense or not, is still unknown. It is clear though, that in the general case, the Neel state is not an eigenstate of the Heisenberg antiferromagnet's Hamiltonian. On the contrary, similar to any other possible quantum state, it is only some linear combination of the Hamiltonian eigenstates. Therefore, the main problem requiring a rigorous investigation is the question of Neel state's stability. In some sense, only for infinitely large lattices, the Neel state becomes the eigenstate of the Hamiltonian and the ground state of the system. Nevertheless, the sublattice structure is observed in experiments on neutron scattering, and, despite certain objections, the actual existence of sublattices is beyond doubt. It should be noted that the spin-wave spectrum of the Heisenberg antiferromagnet differs from the spectrum of the Heisenberg ferromagnet. This point was analyzed thoroughly by Baryakhtar and Popov.<sup>371</sup>

The antiferromagnetic state is characterized by a spatially changing component of magnetization which varies in such a way that the net magnetization of the system is zero. The concept of antiferromagnetism of localized spins which is based on the Heisenberg model and the two-sublattice Neel ground state is relatively well-founded contrary to the antiferromagnetism of delocalized or itinerant electrons. The itinerant-electron picture is the alternative conceptual picture for magnetism.<sup>372</sup> The simplified band model of an antiferromagnet has been formulated by Slater within the single-particle Hartree-Fock approximation. In his approach, he used the "exchange repulsion" to keep electrons with parallel spins away from each other and to lower the Coulomb interaction energy. Some authors consider it as a prototype of the Hubbard model. However, the exchange repulsion was taken proportional to the number of electrons with the same spins only and the energy gap between two subbands was proportional to the difference of electrons with up and down spins. In the antiferromagnetic many-body problem, there is an additional "symmetry broken" aspect. For an antiferromagnet, contrary to ferromagnet, the one-electron Hartree-Fock potential can violate the translational crystal symmetry. The period of the antiferromagnetic spin structure  $L$  is greater than the lattice constant  $a$ . To introduce the two-sublattice picture for itinerant model, one should assume that  $L = 2a$  and that the spins of outer electrons on neighbouring atoms are antiparallel to each other. In other words, the alternating Hartree-Fock potential  $v_{i\sigma} = -\sigma v \exp(iQR_i)$  where  $Q = (\pi/2, \pi/2, \pi/2)$  corresponds to a two-sublattice antiferromagnetic structure. To justify an antiferromagnetic ordering with alternating up and down spin structure, we must admit that in effect two different charge distributions will arise concentrated on atoms of sublattices A and B. This picture accounts well for quasi-localized magnetic behavior.

The earlier theories of itinerant antiferromagnetism were proposed by des Cloizeaux and especially Overhauser.<sup>373,374</sup> Overhauser invented a concept of the static spin density wave which allow the total charge density of the gas to remain spatially uniform. He suggested<sup>373,374</sup> that the mean field ground state of a three

dimensional electron gas is not necessarily a Slater determinant of plane waves. Alternative sets of one-particle states can lead to a lower ground-state energy. Among these alternatives to the plane-wave state are the spin density wave and charge density wave ground states for which the one-electron Hamiltonians have the form

$$H = (p^2/2m) - G(\sigma_x \cos Qz + \sigma_y \sin Qz) \quad (11.8)$$

(spiral spin density wave;  $Q = 2k_F z$ ) and

$$H = (p^2/2m) - 2G \cos(Qr) \quad (11.9)$$

(charge density wave;  $Q = 2k_F z$ ). The periodic potentials in the above expressions lead to a corresponding variation in the electronic spin and charge densities, accompanied by a compensating variation of the background. The effect of Coulomb interaction on the magnetic properties of the electron gas in Overhauser's approach renders the paramagnetic plane-wave state of the free-electron-gas model unstable within the mean field approximation. The long-range components of the Coulomb interaction are most important in creating this instability. It was demonstrated that a nonuniform static spin density wave is lower in energy than the uniform (paramagnetic state) in the Coulomb gas within the mean field approximation for certain electron density.<sup>373-381</sup> The mean field is the simplest approximation but neglects the important dynamical part. To include the dynamics one should take into consideration the correlation effects. The role of correlation corrections which tend to suppress the spin density wave state as well as the role of shielding and screening were not fully clarified. In the Overhauser's approach to itinerant antiferromagnetism the combination of the electronic states with different spins (with pairing of the opposite spins) is used to describe the spin density wave state with period  $Q$ . The first approach is obviously valid only in the simple commensurate two-sublattice case and the latter is applicable to the more general case of an incommensurate spiral spin state. The general spin density wave state has the form

$$\Psi_{p\sigma} = \chi_{p\sigma} \cos(\theta_p/2) + \chi_{p+Q-\sigma} \sin(\theta_p/2) \quad (11.10)$$

The average spin for helical or spiral spin arrangement changes its direction in the  $(x - y)$  plane. For the spiral spin density wave states a spatial variation of magnetization corresponds to  $\vec{Q} = (\pi/a)(1, 1)$ .

The antiferromagnetic phase of chromium and its alloys has been satisfactorily explained in terms of the spin density wave within a two-band model. It is essential to note that chromium becomes antiferromagnetic in a unique manner. The antiferromagnetism is established in a more subtle way from the spins of the itinerant electrons than the magnetism of collective band electrons in metals like iron and nickel. The essential feature of chromium which makes possible the formation of the spin density wave is the existence of "nested" portions of the Fermi surface. The formation of bound electron-hole pairs takes place between particles of opposite spins; the condensed state exhibits the spin density wave.

The problem of a great importance is to understand how broken symmetry can be produced in antiferromagnetism? (see Refs. 230, 375, 382–387) Indeed, it was written in the paper<sup>385</sup> (see also Refs. 230, 375, 383, 384, 386, 387): “One should recall that there are many situations in nature where we do observe a symmetry breaking in the absence of explicit symmetry-breaking fields. A typical example is antiferromagnetism, in which a staggered magnetic field plays the role of symmetry-breaking field. No mechanism can generate a real staggered magnetic field in antiferromagnetic material. A more drastic example is the Bose–Einstein condensation, where the symmetry-breaking field should create and annihilate particles”. The applicability of the Overhauser’s spin density wave concept to highly correlated tight binding electrons on a lattice within the Hubbard model of the correlated lattice fermions was analyzed in Ref. 230. It was shown the importance of the notion of generalized mean fields<sup>207,218</sup> which may arise in the system of correlated lattice fermions to justify and understand the “nature” of the local staggered mean-fields which fix the itinerant antiferromagnetic ordering.

According to Bogoliubov ideas on quasiaverages,<sup>66</sup> in each condensed phase, in addition to the normal process, there is an anomalous process (or processes) which can take place because of the long-range internal field, with a corresponding propagator. Additionally, the Goldstone theorem<sup>127</sup> states that, in a system in which a continuous symmetry is broken (i.e., a system such that the ground state is not invariant under the operations of a continuous unitary group whose generators commute with the Hamiltonian), there exists a collective mode with frequency vanishing, as the momentum goes to zero. For many-particle systems on a lattice, this statement needs a proper adaptation. In the above form, the Goldstone theorem is true only if the condensed and normal phases have the same translational properties. When translational symmetry is also broken, the Goldstone mode appears at a zero frequency but at nonzero momentum, e.g., a crystal and a helical spin-density-wave ordering. The problem of the adequate description of strongly correlated lattice fermions has been studied intensively during the last decade. The microscopic theory of the itinerant ferromagnetism and antiferromagnetism of strongly correlated fermions on a lattice at finite temperatures is one of the important issues of recent efforts in the field. In some papers, the spin-density-wave spectrum was only used without careful and complete analysis of the quasiparticle spectra of correlated lattice fermions. It was of importance to investigate the intrinsic nature of the “symmetry broken” (ferro- and antiferromagnetic) solutions of the Hubbard model at finite temperatures from the many-body point of view. For the itinerant antiferromagnetism the spin density wave spectra were calculated<sup>230</sup> by the irreducible Green functions method,<sup>218</sup> taking into account the damping of quasiparticles. This alternative derivation has a close resemblance to that of the BCS-Bogoliubov theory of superconductivity for transition metals,<sup>218</sup> using the Nambu representation. This aspect of the theory is connected with the concept of broken symmetry, which was discussed in detail for that case. A unified scheme for the construction of generalized mean fields (elastic scattering corrections) and

self-energy (inelastic scattering) in terms of the Dyson equation was generalized in order to include the “source fields”. The “symmetry broken” dynamic solutions of the Hubbard model which correspond to various types of itinerant antiferromagnetism were clarified. This approach complements previous studies of microscopic theory of the Heisenberg antiferromagnet<sup>388</sup> and clarifies the concepts of Neel sublattices for localized and itinerant antiferromagnetism and “spin-aligning fields” of correlated lattice fermions.<sup>389</sup> The advantage of the Green’s function method is the relative ease with which temperature effects may be calculated.

It is necessary to emphasize that there is an intimate connection between the adequate introduction of mean fields and internal symmetries of the Hamiltonian.<sup>389</sup> The anomalous propagators for an interacting many-fermion system corresponding to the ferromagnetic (FM), antiferromagnetic (AFM), and superconducting (SC) long-range ordering are given by

$$\begin{aligned}
 FM : G_{fm} &\sim \langle\langle a_{k\sigma}; a_{k-\sigma}^\dagger \rangle\rangle \\
 AFM : G_{afm} &\sim \langle\langle a_{k+Q\sigma}; a_{k+Q'\sigma'}^\dagger \rangle\rangle \\
 SC : G_{sc} &\sim \langle\langle a_{k\sigma}; a_{-k-\sigma} \rangle\rangle
 \end{aligned}
 \tag{11.11}$$

In the spin-density-wave case, a particle picks up a momentum  $Q - Q'$  from scattering against the periodic structure of the spiral (nonuniform) internal field, and has its spin changed from  $\sigma$  to  $\sigma'$  by the spin-aligning character of the internal field. The long-range-order parameters are:

$$\begin{aligned}
 FM : m &= 1/N \sum_{k\sigma} \langle a_{k\sigma}^\dagger a_{k-\sigma} \rangle \\
 AFM : M_Q &= \sum_{k\sigma} \langle a_{k\sigma}^\dagger a_{k+Q-\sigma} \rangle \\
 SC : \Delta &= \sum_k \langle a_{-k\downarrow}^\dagger a_{k\uparrow} \rangle
 \end{aligned}
 \tag{11.12}$$

It is important to note that the long-range order parameters are functions of the internal field, which is itself a function of the order parameter. There is a more mathematical way of formulating this assertion. According to the paper,<sup>66</sup> the notion “symmetry breaking” means that the state fails to have the symmetry that the Hamiltonian has.

A true breaking of symmetry can arise only if there are infinitesimal “source fields”. Indeed, for the rotationally and translationally invariant Hamiltonian, suitable source terms should be added<sup>389</sup>:

$$\begin{aligned}
 FM : \nu\mu_B H_x &\sum_{k\sigma} a_{k\sigma}^\dagger a_{k-\sigma} \\
 AFM : \nu\mu_B H &\sum_{kQ} a_{k\sigma}^\dagger a_{k+Q-\sigma} \\
 SC : \nu\nu &\sum_k (a_{-k\downarrow}^\dagger a_{k\uparrow}^\dagger + a_{k\uparrow} a_{-k\downarrow})
 \end{aligned}
 \tag{11.13}$$

where  $\nu \rightarrow 0$  is to be taken at the end of calculations.

For example, broken symmetry solutions of the spin-density-wave type imply that the vector  $Q$  is a measure of the inhomogeneity or breaking of translational symmetry. The Hubbard model (9.10) is a very interesting tool for analyzing the symmetry broken concept. It is possible to show that antiferromagnetic state and more complicated states (e.g., ferrimagnetic) can be made eigenfunctions of the self-consistent field equations within an “extended” mean-field approach, assuming that the “anomalous” averages  $\langle a_{i\sigma}^\dagger a_{i-\sigma} \rangle$  determine the behavior of the system on the same footing as the “normal” density of quasi-particles  $\langle a_{i\sigma}^\dagger a_{i\sigma} \rangle$ . It is clear, however, that these “spin-flip” terms break the rotational symmetry of the Hubbard Hamiltonian.<sup>390</sup> Kishore and Joshi<sup>390</sup> discussed the metal-nonmetal transition in ferromagnetic as well as in antiferromagnetic systems having one electron per atom and described by the Hamiltonian which consists of one particle energies of electrons, intra-atomic Coulomb, and interatomic Coulomb and exchange interactions between electrons. It was found that the anomalous correlation functions corresponding to spin flip processes in the Hartree–Fock approximation give rise to the metal-nonmetal transition. The nature of phase transition in ferromagnetic and antiferromagnetic systems was compared and clarified in their study.

For the single-band Hubbard Hamiltonian, the averages  $\langle a_{i-\sigma}^\dagger a_{i,\sigma} \rangle = 0$  because of the rotational symmetry of the Hubbard model. The inclusion of “anomalous” averages leads to the so-called generalized mean field approximation. This type of approximation was used sometimes also for the single-band Hubbard model for calculating the density of states. For this aim, the following definition of generalized mean field approximation

$$n_{i-\sigma} a_{i\sigma} \approx \langle n_{i-\sigma} \rangle a_{i\sigma} - \langle a_{i-\sigma}^\dagger a_{i\sigma} \rangle a_{i-\sigma} \tag{11.14}$$

was used. Thus, in addition to the standard mean field term, the new so-called “spin-flip” terms are retained. This example clearly shows that the structure of mean field follows from the specificity of the problem and should be defined in a proper way. So, one needs a properly defined effective Hamiltonian  $H_{\text{eff}}$ . In the paper<sup>230</sup> we thoroughly analyzed the proper definition of the irreducible Green functions which includes the “spin-flip” terms for the case of itinerant antiferromagnetism of correlated lattice fermions. For the single-orbital Hubbard model, the definition of the irreducible part should be modified in the following way:

$$\begin{aligned} {}^{(ir)} \langle\langle a_{k+p\sigma} a_{p+q-\sigma}^\dagger a_{q-\sigma} a_{k\sigma}^\dagger \rangle\rangle_\omega &= \langle\langle a_{k+p\sigma} a_{p+q-\sigma}^\dagger a_{q-\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega \\ &\quad - \delta_{p,0} \langle n_{q-\sigma} \rangle G_{k\sigma} - \langle a_{k+p\sigma} a_{p+q-\sigma}^\dagger \rangle \langle\langle a_{q-\sigma} | a_{k\sigma}^\dagger \rangle\rangle_\omega. \end{aligned} \tag{11.15}$$

From this definition, it follows that this way of introduction of the irreducible Green functions broadens the initial algebra of operators and the initial set of the Green functions. This means that the “actual” algebra of operators must include the spin-flip terms from the beginning, namely:  $(a_{i\sigma}, a_{i\sigma}^\dagger, n_{i\sigma}, a_{i\sigma}^\dagger a_{i-\sigma})$ . The corresponding

initial Green function will be of the form

$$\begin{pmatrix} \langle\langle a_{i\sigma} | a_{j\sigma}^\dagger \rangle\rangle & \langle\langle a_{i\sigma} | a_{j-\sigma}^\dagger \rangle\rangle \\ \langle\langle a_{i-\sigma} | a_{j\sigma}^\dagger \rangle\rangle & \langle\langle a_{i-\sigma} | a_{j-\sigma}^\dagger \rangle\rangle \end{pmatrix}.$$

With this definition, one introduces the so-called anomalous (off-diagonal) Green functions which fix the relevant vacuum and select the proper symmetry broken solutions. The theory of the itinerant antiferromagnetism<sup>230</sup> was formulated by using sophisticated arguments of the irreducible Green functions method in complete analogy with our description of the Heisenberg antiferromagnet at finite temperatures.<sup>388</sup> For the two-sublattice antiferromagnet we used the matrix Green function of the form

$$\hat{G}(k; \omega) = \begin{pmatrix} \langle\langle S_{ka}^+ | S_{-ka}^- \rangle\rangle & \langle\langle S_{ka}^+ | S_{-kb}^- \rangle\rangle \\ \langle\langle S_{kb}^+ | S_{-ka}^- \rangle\rangle & \langle\langle S_{kb}^+ | S_{-kb}^- \rangle\rangle \end{pmatrix}. \quad (11.16)$$

Here, the Green functions on the main diagonal are the usual or normal Green functions, while the off-diagonal Green functions describe contributions from the so-called anomalous terms, analogous to the anomalous terms in the BCS-Bogoliubov superconductivity theory. The anomalous (or off-diagonal) average values in this case select the vacuum state of the system precisely in the form of the two-sublattice Neel state.<sup>218</sup> The investigation of the existence of the antiferromagnetic solutions in the multiorbital and two-dimensional Hubbard model is an active topic of research. Some complementary to the present study aspects of the broken symmetry solutions of the Hubbard model were considered in Refs. 391–397.

### 11.3. *Bose systems*

A significant development in the past decades have been experimental and theoretical studies of the Bose systems at low temperatures.<sup>320,321,398–416</sup> Any state of matter is classified according to its order, and the type of order that a physical system can possess is profoundly affected by its dimensionality. Conventional long-range order, as in a ferromagnet or a crystal, is common in three-dimensional systems at low temperature. However, in two-dimensional systems with a continuous symmetry, true long-range order is destroyed by thermal fluctuations at any finite temperature. Consequently, for the case of identical bosons, a uniform two-dimensional fluid cannot undergo Bose–Einstein condensation, in contrast to the three-dimensional case. However, the two-dimensional system can form a “quasi-condensate” and become superfluid below a finite critical temperature. Generally, inter-particle interaction is responsible for a phase transition. But Bose–Einstein condensation type of phase transition occurs entirely due to the Bose–Einstein statistics. The typical situation is a many-body system made of identical bosons, e.g., atoms carrying an integer total angular momentum. To proceed, one must construct the ground state. The simplest possibility to do so occurs when bosons are non-interacting. In this case, the ground state is simply obtained by putting all



bosons in the lowest energy single particle state. If the number of bosons is taken to be  $N$ , then the ground state is  $|N, 0, \dots\rangle$  with energy  $N\varepsilon_0$ . This straightforward observation underlies the phenomenon of Bose–Einstein condensation: A finite or macroscopic fraction of bosons has the single-particle energy  $\varepsilon_0$  below the Bose–Einstein transition temperature  $T_{BE}$  in the thermodynamic limit of infinite volume  $V$  but finite particle density. From a conceptual point of view, it is more fruitful to associate Bose–Einstein condensation with the phenomenon of spontaneous symmetry breaking of a continuous symmetry than with macroscopic occupation of a single-particle level. The continuous symmetry in question is the freedom in the choice of the global phase of the many particle wave functions. This symmetry is responsible for total particle number conservation. In mathematical terms, the vanishing commutator  $[H, N_{\text{tot}}]$  between the total number operator  $N_{\text{tot}}$  and the single-particle Hamiltonian  $H$  implies a global  $U(1)$  gauge symmetry. Spontaneous symmetry breaking in Bose–Einstein condensates was studied in Refs. 402, 413. The structure of the many-particle wavefunction for a pair of ideal gas Bose–Einstein condensates  $a, b$  in the number eigenstate  $|N_a N_b\rangle$  was analyzed.<sup>413</sup> It was found that the most probable many-particle position or momentum measurement outcomes break the configurational phase symmetry of the state. Analytical expressions for the particle distribution and current density for a single experimental run are derived and found to display interference. Spontaneous symmetry breaking is thus predicted and explained here simply and directly as a highly probable measurement outcome for a state with a definite number of particles. Lieb and co-authors<sup>402</sup> presented a general proof of spontaneous breaking of gauge symmetry as a consequence of Bose–Einstein condensation. The proof is based on a rigorous validation of Bogoliubov's  $c$ -number substitution for the  $\vec{k} = 0$  mode operator  $a_0$ .

It has been conclusively demonstrated that two-dimensional systems of interacting bosons do not possess long-range order at finite temperatures.<sup>407,408</sup> Gunther, Imry and Bergman<sup>410</sup> show that the one- and two-dimensional ideal Bose gases undergo a phase transition if the temperature is lowered at constant pressure. At the pressure-dependent transition temperature  $T_c(P)$  and in their thermodynamic limit, the specific heat at constant pressure  $c_p$  and the particle density  $n$  diverge, the entropy  $S$  and specific heat at constant volume  $c_v$  fall off sharply but continuously to zero, and the fraction of particles in the ground state  $N_0/N$  jumps discontinuously from zero to one. This Bose–Einstein condensation provides a remarkable example of a transition which has most of the properties of a second-order phase transition, except that the order parameter is discontinuous. The nature of the condensed state is described in the large but finite  $N$  regime, and the width of the transition region was estimated. The effects of interactions in real one- and two-dimensional Bose systems and the experiments on submonolayer helium films were discussed.

A stronger version of the Bogoliubov inequality was used by Roepstorff<sup>412</sup> to derive an upper bound for the anomalous average  $|\langle a(x) \rangle|$  of an interacting nonrelativistic Bose field  $a(x)$  at a finite temperature. This bound is  $|\langle a(x) \rangle|^2 < \rho R$ , where

$R$  satisfies  $1 - R = (RT/2T_c)^{D/2}$ , with  $D$  the dimensionality, and  $T_c$  the critical temperature in the absence of interactions. The formation of nonzero averages is closely related to the Bose–Einstein condensation and  $|\langle a(x) \rangle|^2$  is often believed to coincide with the mean density  $\rho_0$  of the condensate. The author has found nonrigorous arguments supporting the inequality  $\rho_0 \leq |\langle a(x) \rangle|^2$ , which parallels the result of Griffiths in the case of spin systems.

Bose–Einstein condensation continues to be a topic of high experimental and theoretical interest.<sup>320,321,398–401,403–406,415,417,418</sup> The remarkable realization of Bose–Einstein condensation of trapped alkali atoms has created an enormous interest in the properties of the weakly interacting Bose gas. Although the experiments are carried out in magnetic and optical harmonic traps, the homogeneous Bose gas has also received renewed interest. The homogeneous Bose gas is interesting in its own right, and it was proved useful to go back to this somewhat simpler system to gain insight that carries over to the trapped case. Within the last twenty years a lot of works were done on this topic.

The pioneering paper by Bogoliubov in 1947 was the starting point for a microscopic theory of superfluidity.<sup>250</sup> Bogoliubov found the non-perturbative solution for a weakly interacting gas of bosons. The main step in the diagonalization of the Hamiltonian is the famous Bogoliubov transformation, which expresses the elementary excitations (or quasiparticles) with momentum  $q$  in terms of the free particle states with momentum  $+q$  and  $-q$ . For small momenta, the quasiparticles are a superposition of  $+q$  and  $-q$  momentum states of free particles. Recently, experimental observation of the Bogoliubov transformation for a Bose–Einstein condensed gas became possible.<sup>399,403,419,420</sup> Following the theoretical suggestion in Ref. 419, authors of paper<sup>420</sup> observed such superposition states by first optically imprinting phonons with wavevector  $q$  into a Bose–Einstein condensate and probing their momentum distribution using Bragg spectroscopy with a high momentum transfer. By combining both momentum and frequency selectivity, they were able to “directly photograph” the Bogoliubov transformation.<sup>420</sup>

It is interesting to note that Sannino and Tuominen<sup>421</sup> reconsidered the spontaneous symmetry breaking in gauge theories via Bose–Einstein condensation. They proposed a mechanism leading naturally to spontaneous symmetry breaking in a gauge theory. The Higgs field was assumed to have global and gauged internal symmetries. Authors associated a nonzero chemical potential with one of the globally conserved charges commuting with all the gauge transformations. This induces a negative mass squared for the Higgs field, triggering the spontaneous symmetry breaking of the global and local symmetries. The mechanism is general and they tested the idea for the electroweak theory in which the Higgs sector is extended to possess an extra global Abelian symmetry. With this symmetry they associated a nonzero chemical potential. The Bose–Einstein condensation of the Higgs bosons leads, at the tree level, to modified dispersion relations for the Higgs field, while the dispersion relations of the gauge bosons and fermions remain undisturbed.

The latter were modified through higher order corrections. Authors have computed some corrections to the vacuum polarizations of the gauge bosons and fermions. To quantify the corrections to the gauge boson vacuum polarizations with respect to the standard model they considered the effects on the  $T$  parameter. Sannino and Tuominen derived also the one loop modified fermion dispersion relations. It is worth noting that Batista and Nussinov<sup>214</sup> extended Elitzur's theorem<sup>83</sup> to systems with symmetries intermediate between global and local. In general, their theorem formalizes the idea of dimensional reduction. They applied the results of this generalization to many systems that are of current interest. These include liquid crystalline phases of quantum Hall systems, orbital systems, geometrically frustrated spin lattices, Bose metals, and models of superconducting arrays.

## 12. Conclusion and Discussion

In this paper, we have reviewed several fundamental concepts of the modern quantum physics which manifest the operational ability of the notion of symmetry: broken symmetry, quasiaverages, quantum protectorate, emergence, etc. We demonstrated their power of the unification of various complicated phenomena and presented certain evidences for their utility and predictive ability. Broadly speaking, these concepts are unifying and profound ideas "that illuminate our understanding of nature". In particular, the Bogoliubov's method of quasiaverages gives the deep foundation and clarification of the concept of broken symmetry. It makes the emphasis on the notion of a degeneracy and plays an important role in equilibrium statistical mechanics of many-particle systems. According to that concept, infinitely small perturbations can trigger macroscopic responses in the system if they break some symmetry and remove the related degeneracy (or quasidegeneracy) of the equilibrium state. As a result, they can produce macroscopic effects even when the perturbation magnitude tends to zero, provided that it happens after passing to the thermodynamic limit. This approach has penetrated, directly or indirectly, many areas of the contemporary physics as it was shown in the paper by Y. Nambu<sup>103</sup> and in the present review. Nambu emphasized rightly the "cross fertilization" effect of the notion of broken symmetry. The same words could be said about the notion of quasiaverages. It was shown recently that the notion of broken symmetry can be adopted and applied to quantum mechanical problems.<sup>120,124,334,368</sup> Thus it gives a method to approach a many body problem from an intrinsic point of view.<sup>117</sup> On the other hand, it is clear that only a thorough experimental and theoretical investigation of quasiparticle many-body dynamics of the many particle systems can provide the answer on the relevant microscopic picture.<sup>218</sup> As is well-known, Bogoliubov was first to emphasize the importance of the time scales in the many-particle systems thus anticipating the concept of emergence of macroscopic irreversible behavior starting from the reversible dynamic equations.<sup>422-424</sup> More recently, it has been possible to go one step further. This step leads to a much deeper understanding of the relations between microscopic dynamics and

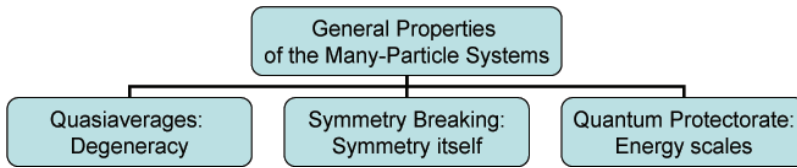


Fig. 1. Schematic form of the interrelation of three profound concepts: quasiaverages, broken symmetry and quantum protectorate.

macroscopic behavior.<sup>60,202,204</sup> It is also worth noticing that the notion of quantum protectorate<sup>60,61</sup> complements the concepts of broken symmetry and quasiaverages by making emphasis on the hierarchy of the energy scales of many-particle systems (see Fig. 1). In an indirect way, these aspects arose already when considering the scale invariance and spontaneous symmetry breaking.<sup>118</sup> D. N. Zubarev showed<sup>69</sup> that the concepts of symmetry breaking perturbations and quasiaverages play an important role in the theory of irreversible processes as well. The method of the construction of the nonequilibrium statistical operator<sup>69,70,218</sup> becomes especially deep and transparent when it is applied in the framework of the quasiaverage concept. The main idea of this approach was to consider infinitesimally small sources breaking the time-reversal symmetry of the Liouville equation,<sup>425</sup> which become vanishingly small after a thermodynamic limiting transition.

To summarize, the Bogoliubov's method of quasiaverages plays a fundamental role in equilibrium and nonequilibrium statistical mechanics and quantum field theory and is one of the pillars of modern physics. It will serve for the future development of physics<sup>426</sup> as an invaluable tool. All the methods developed by N. N. Bogoliubov are and will remain the important core of a theoretician's toolbox, and of the ideological basis behind this development.

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