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SESSION "STATISTICAL MECHANICS, KINETICS AND QUANTUM THEORY OF CONDENSED MATTER"

Symmetry Breaking, Quantum Protectorate and Quasiaverages in Condensed Matter Physics[1, 2]

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Abstract—Substantial progress in the understanding of the spontaneously broken symmetry concept is connected with Bogoliubov's fundamental ideas about quasiaverages. The development and applications of the method of quasiaverages, formulated by N. N. Bogoliubov, to quantum statistical mechanics and to quantum solid state theory and, in particular, to quantum theory of magnetism, are discussed. Some physical implications involved in a new concept, termed the quantum protectorate, are considered.

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It is well known that symmetry principles play a crucial role in physics. The theory of symmetry is a basic tool for understanding and formulating the fundamental notions of physics. 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 important aspect of the degeneracy problem in quantum mechanics when a system possess 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. 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 [1, 2, 3, 4, 5]. Studies of degenerate systems led Bogoliubov in 1960–1961 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 (1, 2, 3, 4, 5]. The very elegant work of N.N. Bogoliubov [2] has been of great importance for a deeper understanding of phase transitions, superfluidity [6] and superconductivity [7], quantum theory of magnetism [8] and other fields of equilibrium and nonequillbrium statistical mechanics [2, 3, 4, 5, 9, 10]. The Bogoliubov's idea of *quasiaverages* is an essential conceptual advance of modern physics.

According to F. Wilczek [11], "the primary goal of fundamental physics is to discover profound concepts that illuminate our understanding of nature." The chief purposes of this report are to demonstrate the connection and interrelation of three complementary conceptual advances (or "profound concepts") of the many-body physics, namely the broken symmetry [12, 13], quasiaverages and quantum protectorate [14], and to try to show explicitly that those concepts, though different in details, have a certain common features. The detailed analysis was carried out of the idea of quantum protectorate [14] in the context of quantum theory of magnetism [15]. This idea reveals the essential difference in the behaviour of the complex many-body systems at the low-energy and high-energy scales. It was suggested [15] 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 [15]. We argue 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** behaviour of electrons. We formulated a criterion of what basic picture describes best this dual behaviour. The main suggestion is that quasi-particle excitation spectra might provide distinctive signatures and good criteria for the appropriate choice of the relevant model. A broad class of the problems of con-

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densed matter physics [16] in the fields of the magnetism and superconductivity of complex materials were reconsidered in relation to these ideas.

In the work of N.N. Bogoliubov "Quasiaverages in Problems of Statistical Mechanics" the innovative notion of *quasiaverage* [2] was introduced and applied to various problem 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 [12]. 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 findings 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 have always the degenerate case due to existence of the additive conservation laws. The traditional approach to quantum statistical mechanics [5] 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 ρ. For an operator $\mathcal{A}$ corresponding to some physical quantity A the average value of A will be given as

$$\langle A\rangle_H = \mathrm{Tr}\rho A;\ \ \rho = \exp^{-\beta H}/\mathrm{Tr}\exp^{-\beta H}. \tag{1}$$

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

The core of the problem lies in establishing the existence of a thermodynamic limit (such as $N/V =$ const, $V \longrightarrow \infty$, $N =$ number of degrees of freedom, $V =$ volume) and its evaluation for the quantities of interest. 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 Schroedinger picture) have the same energy, there is a degeneracy. 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 (1) 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 $=$ $H + \nu(\vec{e}\cdot\vec{M})$, $(\nu \longrightarrow 0)$. 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 [2], the quasiaverage of a dynamical quantity A for the system with the Hamiltonian $H_{\nu\vec{e}}$ is defined as the limit

$$\lessdot A \gtrdot = \lim_{\nu\to 0}\langle A\rangle_{\nu\vec{e}}, \tag{2}$$

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 ν, which vanish as $\nu \longrightarrow 0$ after passage to the thermodynamic limit $V \longrightarrow \infty$. 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

$$\langle A\rangle = \int \lessdot A \gtrdot d\vec{e}. \tag{3}$$

According to definition (3), 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 [5]. 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 [2] 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, 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 ν. 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. Thus the quasiaverages do not follow the same selection rules as those which govern ordinary averages, due to their invariance with regard to the spin rotation group. It is clear that 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 question of symmetry breaking within the localized and band models of antiferromagnets was studied by the author of this report in [15, 16, 17]. It has been found there that the concept of spontaneous symmetry breaking in the band model of magnetism is much more complicated than in the localized model [17]. In the framework of the band model of magnetism one has to additionally consider the so called anomalous propagators of the form [17]

$$\mathrm{FM}: G_{fm} \sim \langle\langle a_{k\sigma}; a^{\dagger}_{k-\sigma}\rangle\rangle,$$

$$\mathrm{AFM}: G_{afm} \sim \langle\langle a_{k+Q\sigma}; a^{\dagger}_{k+Q'\sigma'}\rangle\rangle.$$

In the case of the band antiferromagnet the ground state of the system corresponds to a spin-density wave (SDW), where a particle scattered on the internal inhomogeneous periodic field gains the momentum $Q - Q'$ and changes its spin: $\sigma \longrightarrow \sigma'$. The long-range order parameters are defined as follows:

$$\mathrm{FM}: m = 1/N\sum_{k\sigma}\langle a^{\dagger}_{k\sigma}a_{k-\sigma}\rangle, \tag{4}$$

$$\mathrm{AFM}: M_Q = \sum_{k\sigma}\langle a^{\dagger}_{k\sigma}a_{k+Q-\sigma}\rangle. \tag{5}$$

It is important to stress, that the long-range order parameters here are functionals of the internal field, which in turn is a function of the order parameter. Thus, in the cases of Hamiltonians of band ferro- and antiferromagnetics one has to add the following infinitesimal sources removing the degeneracy:

$$\mathrm{FM}: \nu\mu_B H_x\sum_{k\sigma}a^{\dagger}_{k\sigma}a_{k-\sigma}, \tag{6}$$

$$\mathrm{AFM}: \nu\mu_B H\sum_{kQ}a^{\dagger}_{k\sigma}a_{k+Q-\sigma}. \tag{7}$$

Here, $\nu \longrightarrow 0$ after the usual in statistical mechanics infinite-volume limit $V \longrightarrow \infty$. The ground state in the form of a spin-density wave was obtained for the first time by Overhauser. There, the vector $\vec{Q}$ is a measure of inhomogeneity or translation symmetry breaking in the system. The analysis performed by various authors showed that the antiferromagnetic and more complicated states (for instance, ferrimagnetic) can be described in the framework of a generalized mean-field approximation. In doing that we have to take into account both the normal averages $\langle a^{\dagger}_{i\sigma}a_{i\sigma}\rangle$ and the anomalous averages $\langle a^{\dagger}_{i\sigma}a_{i-\sigma}\rangle$. It is clear that the anomalous terms break the original rotational symmetry of the Hubbard Hamiltonian. Thus, the generalized mean-field's approximation has the following form $n_{i-\sigma}a_{i\sigma} \simeq \langle n_{i-\sigma}\rangle a_{i\sigma} - \langle a^{\dagger}_{i-\sigma}a_{i\sigma}\rangle a_{i-\sigma}$. A self-consistent theory of band antiferromagnetism was developed by the author of this report using the method of the irreducible Green functions [16, 17]. The following definition of the irreducible Green functions was used:

$$\begin{aligned}&{}^{ir}\langle\langle a_{k+p\sigma}a^{\dagger}_{p+q-\sigma}a_{q-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega}\\ &= \langle\langle a_{k+p\sigma}a^{\dagger}_{p+q-\sigma}a_{q-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega} - \delta_{p,0}\langle n_{q-\sigma}\rangle G_{k\sigma}\\ &\quad - \langle a_{k+p\sigma}a^{\dagger}_{p+q-\sigma}\rangle\langle\langle a_{q-\sigma}|a^{\dagger}_{k\sigma}\rangle\rangle_{\omega}.\end{aligned} \tag{8}$$

The algebra of relevant operators must be chosen as follows ($a_{i\sigma}$, $a^{\dagger}_{i\sigma}$, $n_{i\sigma}$, $a^{\dagger}_{i\sigma}a_{i-\sigma}$). The corresponding initial GF will have the following matrix structure

$$\mathcal{G}_{AFM} = \begin{pmatrix} \langle\langle a_{i\sigma}|a^{\dagger}_{j\sigma}\rangle\rangle & \langle\langle a_{i\sigma}|a^{\dagger}_{j-\sigma}\rangle\rangle \\ \langle\langle a_{i-\sigma}|a^{\dagger}_{j\sigma}\rangle\rangle & \langle\langle a_{i-\sigma}|a^{\dagger}_{j-\sigma}\rangle\rangle \end{pmatrix}.$$

The off-diagonal terms select the vacuum state of the band's antiferromagnet in the form of a spin-density wave. It is necessary to stress that the problem of the band's antiferromagnetism is quite involved, and the construction of a consistent microscopic theory of this phenomenon remains a topical problem. The "quantum protectorate" concept was formulated in the paper [14]. Its authors R. Laughlin and D. Pines discuss the most fundamental principles of matter description in the widest sense of this word. The authors formulate their main thesis: emergent physical phenomena, which are regulated by higher physical principles, have a certain property, typical for these phenomena only. This property is their insensitivity to microscopic description. For instance, 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. There are many other examples [14]. 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 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 [15, 16] devoted to comparative analysis of localized and band models of quantum theory of magnetism. It was shown there, that the low-energy spectrum of magnetic excitations in the magnetically-ordered solid bodies corresponds to a hydrodynamic pole ($\vec{k}$, $\omega \longrightarrow 0$) in the generalized spin susceptibility χ, 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 $\vec{k}$, $\omega \longrightarrow 0$, 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 [15], 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.

To summarize, 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 is tend to zero, provided that happens after passing to the thermodynamic limit. The notion of quantum protectorate complements the concepts of broken symmetry and quasiaverages by making emphasis on the hierarchy of the energy scales of many-particle systems. D.N. Zubarev showed [9] 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 [9, 10, 16] 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, which become vanishingly small after a thermodynamic limiting transition. Therefore the method of quasiaverages plays a fundamental role in equilibrium and nonequilibrium statistical mechanics and is one of the pillars of modern physics.

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