Extended ensemble theory, spontaneous symmetry breaking, and phase transitions

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Received 6 May 2006
Accepted 22 August 2006
Published 14 September 2006

Abstract. In this paper, as a personal review, we suppose a possible extension of Gibbs ensemble theory so that it can provide a reasonable description of phase transitions and spontaneous symmetry breaking. The extension is founded on three hypotheses, and can be regarded as a microscopic edition of the Landau phenomenological theory of phase transitions. Within its framework, the stable state of a system is determined by the evolution of order parameter with temperature according to such a principle that the entropy of the system will reach its minimum in this state. The evolution of order parameter can cause a change in representation of the system Hamiltonian; different phases will realize different representations, respectively; a phase transition amounts to a representation transformation. Physically, it turns out that phase transitions originate from the automatic interference among matter waves as the temperature is cooled down. Typical quantum many-body systems are studied with this extended ensemble theory. We regain the Bardeen–Cooper–Schrieffer solution for the weak-coupling superconductivity, and prove that it is stable. We find that negative-temperature and laser phases arise from the same mechanism as phase transitions, and that they are unstable. For the ideal Bose gas, we demonstrate that it will produce Bose–Einstein condensation (BEC) in the thermodynamic limit, which confirms exactly Einstein’s deep physical insight. In contrast, there is no BEC either within the phonon gas in a black body or within the ideal photon gas in a solid body. We prove that it is not admissible to quantize the Dirac field by using Bose–Einstein statistics. We show that a structural phase transition belongs physically to the BEC happening in configuration space, and that a double-well anharmonic system will undergo a structural phase transition.
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at a finite temperature. For the $O(N)$-symmetric vector model, we demonstrate that it will yield spontaneous symmetry breaking and produce Goldstone bosons; and if it is coupled with a gauge field, the gauge field will obtain a mass (Higgs mechanism). Also, we show that an interacting Bose gas is stable only if the interaction is repulsive. For the weak interaction case, we find that the BEC is a ‘$\lambda$-transition’ and its transition temperature can be lowered by the repulsive interaction. In connection with liquid $^4$He, it is found that the specific heat at constant pressure $C_P$ will show a $T^3$ law at low temperatures, which is in agreement with the experiment. If the system is further cooled down, the theory predicts that $C_P$ will vanish linearly as $T \to 0$, which is anticipating experimental verifications.

**Keywords:** Bose Einstein condensation (theory), quantum phase transitions (theory), exact results

**ArXiv ePrint:** cond-mat/0512175

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1. Introduction

1.1. The problem of Gibbs ensemble theory

Since Gibbs [1] established the ensemble theory of statistical mechanics, there has arisen the problem as to whether or not it has the ability to describe phase transitions [2].

Let us investigate the problem through the famous example, i.e., conventional low-$T_c$ superconductivity, which can be described by the so-called Bardeen–Cooper–Schrieffer (BCS) Hamiltonian [3]–[5],

$$H(c) = \sum_k \epsilon(k)(c_{k\uparrow}^\dagger c_{k\uparrow} + c_{-k\downarrow}^\dagger c_{-k\downarrow}) - g \sum_{k,k'} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k\downarrow} c_{k\uparrow},$$  \hspace{1cm} (1.1)

where $\epsilon(k)$ denotes the energy relative to the Fermi level, $g > 0$ the coupling strength, $c_{k\uparrow}$ and $c_{k\downarrow}$ ($c_{k\uparrow}^\dagger$ and $c_{k\downarrow}^\dagger$) the destruction (creation) operators for the electrons with up and down spins, respectively. Here, the notation $H(c)$ expresses that the Hamiltonian is a function of $c_{k\uparrow}$, $c_{k\downarrow}$, $c_{k\uparrow}^\dagger$, and $c_{k\downarrow}^\dagger$.

For BCS superconductivity, what is most important physically is that the Hamiltonian $H(c)$ will remain invariant under the transformation,

$$G(\vartheta,c)H(c)G^\dagger(\vartheta,c) = H(c),$$ \hspace{1cm} (1.2)

where

$$G(\vartheta,c) = e^{-i\vartheta \sum_k (c_{k\uparrow}^\dagger c_{k\downarrow} + c_{k\downarrow}^\dagger c_{k\uparrow})}, \quad \vartheta \in [0, 2\pi).$$ \hspace{1cm} (1.3)

This invariance is known as gauge symmetry. As a direct consequence of this symmetry, one has

$$\langle c_{-k\downarrow} c_{k\uparrow} \rangle = \text{Tr} (c_{-k\downarrow} c_{k\uparrow} \rho(H(c))) = 0,$$ \hspace{1cm} (1.4)

where $\langle \cdots \rangle$ denotes the Gibbs ensemble average with respect to the Hamiltonian $H(c)$, and

$$\rho(H) = \frac{e^{-\beta H}}{\text{Tr}(e^{-\beta H})}$$ \hspace{1cm} (1.5)

is the statistical density operator, where $\beta = 1/(k_B T)$, with $k_B$ and $T$ being the Boltzmann constant and temperature, respectively. To prove equation (1.4), it is sufficient to heed that

$$G\left(\frac{\pi}{2},c \right) c_{-k\downarrow} c_{k\uparrow} G^\dagger\left(\frac{\pi}{2},c \right) = -c_{-k\downarrow} c_{k\uparrow}.$$ \hspace{1cm} (1.6)

Equation (1.4) indicates that the electron-pair amplitude $\langle c_{-k\downarrow} c_{k\uparrow} \rangle$ can never become nonzero according to Gibbs ensemble theory; in other words, superconductivity cannot happen for the BCS Hamiltonian of equation (1.1) within Gibbs ensemble theory, no
matter how low the temperature is. This proves definitely that Gibbs ensemble theory has no ability to describe phase transitions.

Even so, it is still hoped to make as little as possible modification to Gibbs theory so that it could describe phase transitions. Up to now, there have been two kinds of modification: they both arise from the theoretical studies on the so-called Ising model [6], and have become the popular and predominant beliefs about phase transitions in the current world of statistical physics.

The first is to introduce the thermodynamic limit at the end of calculation [7]–[14], that is,

$$\langle c_{-k}|c_k \rangle = \lim_{V \to +\infty} \text{Tr} \left( c_{-k}|c_k \rangle \rho(H(c)) \right),$$

(1.7)

where \( \lim_{V \to +\infty} \) means to take the thermodynamic limit \( (V \to +\infty, N \to +\infty, and N/V = constant) \) after performing the trace. Because

$$\text{Tr} \left( c_{-k}|c_k \rangle \rho(H(c)) \right) = 0,$$

(1.8)

irrespective of the magnitudes of \( V, N, and N/V \) (\( H(c) \) is invariant under gauge transformation, and that is true independently of \( V, N, and N/V \), namely, the gauge symmetry has nothing to do with \( V, N, and N/V \)), one has

$$\lim_{V \to +\infty} \text{Tr} \left( c_{-k}|c_k \rangle \rho(H(c)) \right) = 0.$$

(1.9)

Therefore, this kind of modification cannot make Gibbs ensemble theory have the ability to describe phase transitions. Indeed, the thermodynamic limit is important for calculating the statistical average of observables, but itself alone is insufficient to act as the physical criterion for phase transitions.

The second is to introduce both the thermodynamic limit and an auxiliary external field [6], [15]–[17],

$$\langle c_{-k}|c_k \rangle = \lim_{\phi \to 0} \lim_{V \to +\infty} \text{Tr} \left( c_{-k}|c_k \rangle \rho \left( H(c) + \sum_k \left( \phi c_{-k}|c_k \rangle + \phi^\dagger c_{k}^\dagger c_{-k}^\dagger \right) \right) \right),$$

(1.10)

where, as pointed out by Huang [17], the limit \( \phi \to 0 \) must be taken after the thermodynamic limit \( V \to +\infty \). The purpose of introducing an auxiliary external field \( \phi \) is to break the gauge symmetry of the system, as can be easily seen from the term

$$\sum_k \left( \phi c_{-k}|c_k \rangle + \phi^\dagger c_{k}^\dagger c_{-k}^\dagger \right).$$

(1.11)

Since the gauge symmetry has been broken with regard to the entire Hamiltonian,

$$H(c) + \sum_k \left( \phi c_{-k}|c_k \rangle + \phi^\dagger c_{k}^\dagger c_{-k}^\dagger \right),$$

(1.12)

in so far as the auxiliary external field \( \phi \) is infinitesimal but nonzero, the trace and the limit \( V \to +\infty \) of equation (1.10) become nonzero. Further, if the limit \( \phi \to 0 \) does not tend to zero, the electron-pair amplitude \( \langle c_{-k}|c_k \rangle \) will become nonzero. One thus concludes that there appear Cooper pairs in the system, and that the system has gone into the superconducting phase. However, this conclusion cannot hold in physics, for the modification suffers from a serious problem: the limit procedure employed by

doi:10.1088/1742-5468/2006/09/P09007
equation (1.10) is physically equivalent to the scenario that an infinitesimal auxiliary external field is first added to the system so as to induce the symmetry of the system to break down, and taken off from the system finally. But, in the actual situation, the inducement of such an external field is unnecessary, the symmetry itself breaks down spontaneously and does not need any help from an external force. Anyhow, this kind of modification contains unphysical operations, and thus cannot be accepted in principle.

Here, it is also significant and worthwhile to give a brief discussion of the two-dimensional Ising model because it can be solved exactly within the two modifications,

\[ H_I = -J \sum_{\langle ij \rangle} s_is_j, \]  

where \( s_i = \pm 1 \) denotes the spin variable on site \( i \), the symbol \( \langle ij \rangle \) means that the sites \( i \) and \( j \) are nearest neighbours, and \( J > 0 \) is the exchange coupling between a nearest-neighbour pair of spins.

As is well known, Onsager [7] proved rigorously that the specific heat of the Ising Hamiltonian \( H_I \) is singular at \( T = T_c > 0 \) within the first modification of Gibbs ensemble theory. It hints that the system might undergo a paramagnetic–ferromagnetic phase transition at \( T_c \) in the thermodynamic limit. However, just as equations (1.7)–(1.9), the magnetization \( m \),

\[ m = \lim_{N \to \infty} \text{Tr} (s_i \rho (H_I)) = 0, \]  

is always equal to zero due to the fact that the parity symmetry of \( H_I \) with respect to \( s_i = 1 \) and \( s_i = -1 \) has nothing to do with the magnitude of \( N \), where \( N \) represents the total number of sites. Equation (1.14) proves definitely that there is no paramagnetic–ferromagnetic phase transition at any temperature within the first modification of Gibbs ensemble theory even if the specific heat is singular.

The above proof also shows that it cannot be solved within the framework of the first modification whether or not the onset of the singularity at \( T = T_c \) manifests a phase transition. In order to justify that the phenomenon occurring at \( T = T_c \) is a phase transition, Yang [16] went beyond the first modification and turned to the second one, which was, in fact, suggested originally by Ising himself [6] in studying the one-dimensional Ising model. Wonderfully, Yang succeeded in proving rigorously that

\[ m = \lim_{B \to 0} \lim_{N \to \infty} \text{Tr} \left( s_i \rho \left( H_I - B \sum_i s_i \right) \right) \]

where \( B \) stands for an external magnetic field. Mathematically, it seems reasonable to say from equation (1.15) that a paramagnetic–ferromagnetic phase transition will occur at \( T = T_c \). Nevertheless, as pointed out above, equation (1.15) imports unphysical operations from the introduction of the external field \( B \), and this leads to the result that the phase transition will not occur automatically but has to be driven and decided from outside the system, which directly contradicts the basic experimental fact that any phase transition occurs itself spontaneously. Therefore, the second modification, or rather Ising’s criterion,
cannot be used as a physical criterion to justify whether there exists a paramagnetic–ferromagnetic phase transition at $T = T_c$.

It should be stressed again that it is the two rigorous works of [7, 16] that establish the two kinds of modification to the Gibbs ensemble theory.

On all accounts, the two kinds of modification must both be discarded, and it is necessary to modify or extend Gibbs ensemble theory anew. That is just the main purpose of this paper.

Recently, Gibbs ensemble theory has been extended by Tsallis and his followers with the conception of nonextensive entropy [18]–[20], which is under controversy. In this paper, as a personal review, we would like to suppose another possible extension of the Gibbs ensemble theory so that it can provide a reasonable description to phase transitions and spontaneous symmetry breaking (SSB).

1.2. Landau phenomenological theory

Also, there is a macroscopic theory for phase transitions, i.e., Landau phenomenological theory [21].

Phenomenological as it is, Landau theory succeeds in providing a unified picture for all the second-kind phase transitions, e.g., superconductivity, superfluidity, magnetism, and structural phase transitions. Physically, the Landau picture consists of two basic notions: order parameter and variational principle. The order parameter describes the degree of order of the system: it is zero in the disordered phase, and nonzero in the ordered one. The variational principle yields the equation of motion of the order parameter and controls the evolution of order parameter with temperature: a system must arrive at the minimum of Helmholtz or Gibbs free energy in its stable state. According to this picture, a system will evolve with the evolution of its order parameters, and produce phase transitions spontaneously, i.e., without any help or drive from outside the system. In short, the order parameter and variational principle are two characteristics of Landau theory.

On the other hand, Landau pointed out that a phase transition of the second kind reflects physically the change in symmetry of the system: the disordered phase has a higher symmetry than the ordered one. He found that this change in symmetry can be described through the representations of the symmetry group: a phase transition corresponds to a representation transformation, and different phases will realize different representations, respectively. Accordingly, Landau established the relation between the order parameter and the representation. Using this relation, it can be easily determined from the variational principle which representation will be realized at a certain temperature. Representation transformation and spontaneous symmetry breaking are the other two characteristics of Landau theory.

To sum up, a system will select and realize automatically different representations at different temperatures according to the variational principle of the order parameter. That is the mechanism for phase transitions discovered by Landau theory; it crystallizes Landau’s ideas about phase transitions: order parameter, variational principle, representation transformation, and spontaneous symmetry breaking. Theoretically, this mechanism gives a reasonable answer to the problem why a phase transition or SSB can happen at a certain temperature. In applications, it also agrees quite well with various
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phase transitions; its effectiveness and universality are well known to condensed matter physicists. In a word, Landau’s ideas on phase transitions are successful and of great value in physics!

Regrettably, it is impossible to deduce Landau theory from Gibbs ensemble theory because there is no variational principle of order parameter within the latter. This demonstrates again the deficiency of Gibbs ensemble theory. In fact, this deficiency was pointed out by Born and Fuchs [22] early in 1938. In 1937, Mayer [23] published his famous paper on the gas–liquid transition, which is based directly on Gibbs ensemble theory. This work was seriously doubted and questioned by Born and Fuchs [22]: ‘How can the gas molecules ‘know’ when they have to coagulate to form a liquid and solid?’ Obviously, owing to lack of Landau mechanism, it is hard for Gibbs ensemble theory to answer the question posed by Born and Fuchs.

Gibbs ensemble theory should be extended to incorporate the Landau’s ideas so as to describe phase transitions and answer the question posed by Born and Fuchs. That is another intention of this paper.

2. The extended ensemble theory

In order to describe phase transitions and spontaneous symmetry breaking, we shall, as a personal review, extend Gibbs ensemble theory with three hypotheses, which can be stated, taking the BCS superconductivity as an instance, as follows.

(1) The system Hamiltonian is represented by $H'(\phi, c)$,

$$H'(\phi, c) = e^{iD(\phi, c)}H(c)e^{-iD(\phi, c)},$$  \hspace{1cm} (2.1)

where

$$D(\phi, c) = \sum_k (\phi_k c_{-k}^\dagger c_{+k}^\dagger + \phi_{-k}^\dagger c_{k} c_{-k}^\dagger).$$  \hspace{1cm} (2.2)

Here $\phi$ is an internal field of the system, it is also the order parameter for BCS superconductivity. Evidently, $H'(\phi, c)$ is not invariant under the gauge transformation of $G(\vartheta, c)$ as long as $\phi \neq 0$, namely, the gauge symmetry will be broken for $H'(\phi, c)$ if $\phi \neq 0$. From now on, we shall call $D(\phi, c)$ the phase-transition operator, for the sake of convenience.

(2) The statistical average of an observable $F(c)$ is defined as

$$\mathcal{F}(\phi, \beta) = \langle F(c) \rangle = \text{Tr} (F(c)\rho(H'(\phi, c))).$$  \hspace{1cm} (2.3)

We remark that the average is now a function of both temperature and order parameter, which is expressed explicitly by the two arguments of $\mathcal{F}(\phi, \beta)$.

(3) The order parameter $\phi$ is determined by the minimum of the entropy of the system,

$$\delta S = 0,$$  \hspace{1cm} (2.4)

$$\Delta S \geq 0,$$  \hspace{1cm} (2.5)

where $S$ denotes the entropy,

$$S(\phi, \beta) = \langle -\ln (\rho(H(c))) \rangle = -\text{Tr} (\ln (\rho(H(c))) \rho(H'(\phi, c))).$$  \hspace{1cm} (2.6)
As a function of the order parameter, the entropy controls the evolution of state of the system with temperature.

The first hypothesis means that the system Hamiltonian can take different representations at different temperatures; for example, it can take the symmetric representation ($\phi = 0$) at a high temperature, and the asymmetric representation ($\phi \neq 0$) at a low temperature. Which representation it will take is determined by the third hypothesis. After the representation is so determined, the statistical average can be calculated with respect to this representation, as stated in the second hypothesis.

Obviously, the extended theory will reduce to the original one if $\phi = 0$; that is to say, the original theory holds only for the normal phase of the system. The broken-symmetry phase will be described by the extended theory.

Within the framework of the extended ensemble theory, a system will realize different representations of the same system Hamiltonian at different temperatures according to the principle of least entropy with respect to order parameter; this mechanism for phase transitions is, in spirit, the same as that given by Landau phenomenological theory; hence, it can be said that the Landau mechanism has been incorporated into the extended ensemble theory. Also, because the order parameter is an internal field of the system itself, symmetry breaking will occur in a completely spontaneous way rather than being forced by an external field; there is no unphysical operation within the extended theory. In a word, the extended ensemble theory is conceptionally in accordance with Landau’s ideas on phase transitions: order parameter, variational principle, representation transformation, and spontaneous symmetry breaking.

In section 6, we shall show further that phase transitions originate physically from the wave nature of matter.

Now, let us establish the relationship between the extended ensemble theory and thermodynamics; it can be implemented as follows.

First, the internal energy $U$ can be obtained from equation (2.3), replacing $F(c)$ by the Hamiltonian $H(c)$. It is a function of temperature $T$ and volume $V$, that is,

$$U = U(T, V).$$

From the internal energy $U(T, V)$, the specific heat at constant volume, $C_V$, can be calculated through

$$C_V = C_V(T, V) = \left( \frac{\partial U}{\partial T} \right)_V.$$  \hfill (2.8)

Then, we can obtain the thermodynamical entropy $S_{th}$,

$$S_{th} = S_{th}(T, V) = \int_0^T C_V(T', V) \frac{dT'}{T'}. \hfill (2.9)$$

It is worth paying attention to the significant difference between the thermodynamical entropy $S_{th}$ and the statistical entropy $S$ defined in equation (2.6): $S$ measures the degree of order of the system, whereas $S_{th}$ measures the amount of heat absorbed or rejected by the system, i.e., $dQ = T \, dS_{th}$; besides, $S$ contains the basic information of the system: it controls the evolution of state of the system, and as a consequence, $S_{th}$ derives itself from $S$.

Finally, we arrive at

$$F = F(T, V) = U(T, V) - TS_{th}(T, V),$$  \hfill (2.10)
where $F$ is the Helmholtz free energy of the system, with $T$ and $V$ as its natural variables. As a thermodynamic potential of the system, $F$ can generate other thermodynamic quantities. In such a way, the extended ensemble theory connects with thermodynamics.

In the end of this section, let us explain why we choose the BCS model rather than the Ising model as the starting instance to develop the theory for phase transitions and spontaneous symmetry breaking.

As is well known, the Ising model $H_I$ is a classical discrete Hamiltonian. Simple as it is mathematically, it is, however, ill defined from the point of view of physics. On one hand, a classical Hamiltonian, $H = H(q,p)$ where $q$ and $p$ denote the generalized coordinates and momenta of the system, must be continuous in phase space, that is to say, $H(q,p)$ is a continuous function of $q$ and $p$; there does not exist any classical system which corresponds to a discrete Hamiltonian; therefore, $H_I$ does not correspond to a classical system. On the other hand, the discrete quantity $s_i = \pm 1$ is not a quantum operator but a pure integer variable; therefore, $H_I$ does not correspond to a quantum system, either. In a word, the Ising model cannot correspond to any physical system; its solution, whether rigorous or not, has no real physical relevance [2], which was, in fact, realized and pointed out as the ‘Ising disease’ by people early in 1940s and 1950s [2].

To understand that point further, let us first suppose that the Ising model could represent a real physical system, and then analyse the statistical properties of this system in detail. First, if the system is not placed in an external magnetic field, then, according to the Onsager’s solution [6,17], its specific heat will diverge logarithmically at $T = T_c > 0$; however, as indicated by equation (1.14), there appears no spontaneous magnetization below $T_c$, namely, the state of the system will remain nonmagnetic at any temperature, whether $T > T_c$ or $T < T_c$. There is no paramagnetic–ferromagnetic phase transition in the Ising system if it is not placed in an external magnetic field, though its specific heat is singular. That is the first characteristic behaviour of the Ising system. Secondly, if the system is placed in an external magnetic field, then, according to Yang’s solution [16], there will appear an induced magnetization below $T_c$. That is to say, the Ising system will transform from a paramagnetic state at $T > T_c$ into a ferromagnetic state at $T < T_c$ when it is placed in an external magnetic field; here, the transformation is an induced transformation other than a spontaneous phase transition. That is the second characteristic behaviour of the Ising system. In sum, an Ising system will exhibit two distinct behaviours, respectively, depending on whether the system is placed in an external magnetic field or not. It will exhibit the first characteristic behaviour in the case without the application of any external magnetic field and the second one in the case with the application of an external magnetic field. The two behaviours should be checked experimentally with respect to the same physical system. However, such a physical system that can simultaneously show both characteristic behaviours of the Ising model has never been observed and reported experimentally. In other words, the supposed Ising system does not exist in nature at all! That is not surprising; it just reflects the ill definition of the Ising model. Here, it should be pointed out that the solutions of Onsager and Yang are not identical but are essentially different from each other, whether in the sense of mathematics or in the sense of physics: in the limit $B \to 0$, Yang’s solution cannot reduce to Onsager’s solution, as can be easily seen by comparing equations (1.14) and (1.15); they represent the statistical properties of the Ising system with and without the interaction of an external magnetic field, respectively.
Needless to say, an Ising system is completely distinguishable from a real physical system of phase transition. For the latter, the transition happens itself spontaneously, needing no inducement of a corresponding external field. Evidently, this nature of phase transitions is neither the same as the first characteristic behaviour of the Ising system, i.e., a singular specific heat but no phase transition, nor the same as the second characteristic behaviour of the Ising system, i.e., a transformation induced but not spontaneous. There are clear and definite discrepancies between the statistical behaviour of a real physical system of phase transition and those of the Ising system. No phase transition can be described by Ising model. Of course, if one disregards physically the ill definition of the Ising model, the distinction between the solutions of Onsager and Yang, and the discrepancies between the statistical behaviour of a real physical system of phase transition and those of the Ising system, one can simulate some phase transitions and critical phenomena quite well with the Ising model [24]–[32].

Theoretically, the Ising model is ill defined; experimentally, the Ising system does not exist in nature at all. That is the reason why we do not choose it as the starting instance to develop the theory of phase transitions and SSB. As for the BCS model [3]–[5], quite the contrary: it is of high value in theory because it contributes a new quantum concept, i.e., Cooper pairs, which is profound and rather hard to understand theoretically but yet verified exactly by quantized flux experiments. Actually, it is the BCS theory that began our microscopic understanding of phase transitions.

Although Ising’s criterion for phase transitions is problematic in physics, it is indeed very suggestive in mathematics. To some degree, it can be said that the present modification is just equivalent to substituting the external field proposed by Ising with an internal field determined by the system itself, as can be seen from expanding the right-hand side of equation (2.1) to the linear term of $\phi$ and then comparing it with equation (1.12).

3. Application to the ideal Fermi gas

Let us first apply the extended ensemble theory to the ideal Fermi gas. It is the simplest case, and we shall see that this case is exactly solvable.

For the ideal Fermi gas, there is no interaction ($g = 0$); equation (1.1) reduces to

$$H(c) = \sum_k \varepsilon(k)(c_{k\uparrow}c_{k\uparrow} + c_{-k\downarrow}^\dagger c_{-k\downarrow}), \quad (3.1)$$

where $\varepsilon(k) = \hbar^2 k^2 / (2m) - \mu$, with $m$ and $\mu$ being the mass of the fermions and the chemical potential of the system, respectively.

To facilitate the calculation of the entropy, we reformulate equation (2.6) as

$$S(\phi, \beta) = - \text{Tr} \left( \ln \left( \rho \left( H(e^{-iD(\phi,c)c_{c}^{D(\phi,c)}}) \right) \right) \rho(H(c)) \right). \quad (3.2)$$

By use of equation (2.2), we find

$$e^{-iD(\phi,c)} c_{k\uparrow} e^{iD(\phi,c)} = \cos (\theta_k) c_{k\uparrow} + i \sin (\theta_k) e^{-i\phi_k} c_{-k\downarrow}^\dagger \quad (3.3a)$$

$$e^{-iD(\phi,c)} c_{-k\downarrow} e^{iD(\phi,c)} = \cos (\theta_k) c_{-k\downarrow} - i \sin (\theta_k) e^{-i\phi_k} c_{k\uparrow}^\dagger, \quad (3.3b)$$

where $\theta_k = \mid \phi_k \mid$ and $\phi_k = \arg(\phi_k)$. Substituting them into equation (3.2), we have

$$S(\phi, \beta) = \ln \left( \text{Tr}(e^{-\beta H(c)}) \right) + 2\beta \sum_k \varepsilon(k) \left[ \cos^2(\theta_k) f(\varepsilon(k)) + \sin^2(\theta_k) f(-\varepsilon(k)) \right], \quad (3.4)$$

$$\text{doi:10.1088/1742-5468/2006/09/P09007}$$
where
\[ f(\varepsilon) = \frac{1}{e^{\beta \varepsilon} + 1} \quad (3.5) \]
is the Fermi distribution function.

From equations (3.4) and (2.4), it follows that
\[ \sin(2\theta_k) = 0, \quad (3.6) \]
which is the equation of the order parameter. Obviously, this equation has the solutions
\[ \theta_k = 0, \pi/2, \pi, 3\pi/2. \quad (3.7) \]

In addition, one can easily deduce from equation (3.4) that
\[ \Delta S = \sum_k \Delta s_k, \quad (3.8) \]
where
\[ \Delta s_k = \begin{cases} 
\beta \varepsilon(k) \tanh \left( \frac{\beta \varepsilon(k)}{2} \right) [1 - \cos (2\delta \theta_k)] \geq 0, & \theta_k = 0, \text{or } \pi, \\
-\beta \varepsilon(k) \tanh \left( \frac{\beta \varepsilon(k)}{2} \right) [1 - \cos (2\delta \theta_k)] \leq 0, & \theta_k = \pi/2, \text{or } 3\pi/2, 
\end{cases} \quad (3.9) \]
with \( \delta \theta_k \) being the deviation of \( \theta_k \) from the corresponding solution.

For the solution that all \( \theta_k = 0 \) or \( \pi \), we have \( \Delta S \geq 0 \), which meets the requirement of equation (2.5); thereby, this solution corresponds to a stable phase. Observe that the order parameter \( \phi = 0 \) when all \( \theta_k = 0 \); one recognizes immediately that this phase is just the normal phase of the system, which can also be seen from the following equation,
\[ F(\phi, \beta) = \text{Tr} (F(c)\rho(H'(\phi, c))) = \text{Tr} (F(c)\rho(H(c))) = \text{Tr} (e^{-\beta' H(c)}) \quad (3.10) \]
\[ \forall \theta_k = \pi/2, \text{or } 3\pi/2, \]
where \( \beta' = 1/(k_B T') \) with \( T' = -T < 0 \). That is to say, the temperature of the system goes negative. This shows that negative temperatures derive from the same microscopic mechanism as that for phase transitions, so we call this unstable phase the negative-temperature phase. In comparison, the normal phase is said to be the positive-temperature phase \( (T > 0) \). This negative-temperature phase cannot be realized physically because its internal energy is unbounded above.
Apart from the negative-temperature phase, all the other unstable phases are partially negative-temperature phases, which means that the particles of the system are distributed partially among the negative-temperature (single-particle) states, and partially among the positive-temperature (single-particle) states,

\[ \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle = \begin{cases} 
\frac{1}{e^{\beta \epsilon_{\mathbf{k}}(\mathbf{k})} + 1}, & \theta_{\mathbf{k}} = 0, \pi, \\
\frac{1}{e^{\beta' \epsilon_{\mathbf{k}}(\mathbf{k})} + 1}, & \theta_{\mathbf{k}} = \pi/2, 3\pi/2.
\end{cases} \] (3.12)

That is to say, some of the states take 0 or \( \pi \), and the others take \( \pi/2 \) or \( 3\pi/2 \). Each \( \mathbf{k} \) with \( \theta_{\mathbf{k}} = 0 \) or \( \pi \) represents a positive-temperature state, and each \( \mathbf{k} \) with \( \theta_{\mathbf{k}} = \pi/2 \) or \( 3\pi/2 \) represents a negative-temperature state. Because the partially negative-temperature phase is an unstable phase, it can emit photons when particles transfer from a negative-temperature state into a positive-temperature one. Therefore, a partially negative-temperature system can constitute a laser.

To make that point more specific, let us consider a semiconductor that is described by the following Hamiltonian,

\[ H(c) = \sum_{n,\mathbf{k}} \epsilon_n(\mathbf{k}) (c_{n,\mathbf{k}\uparrow}^\dagger c_{n,\mathbf{k}\uparrow} + c_{n,-\mathbf{k}\downarrow}^\dagger c_{n,-\mathbf{k}\downarrow} + c_{n,-\mathbf{k}\downarrow}^\dagger c_{n,\mathbf{k}\uparrow}), \] (3.13)

where \( n \) denotes the energy-band index, \( \epsilon_n(\mathbf{k}) \) the energy of the electrons in the \( n \)th band relative to the Fermi level of the system, and \( c_{n,\mathbf{k}\sigma} \) the annihilation operator of the electrons with momentum \( \mathbf{k} \) and spin \( \sigma \) in the \( n \)th band. Replacing the \( D(\phi, c) \) of equation (2.2) with

\[ D(\phi, c) = \sum_{n,\mathbf{k}} (\phi_{n,\mathbf{k}} c_{n,-\mathbf{k}\downarrow}^\dagger c_{n,\mathbf{k}\uparrow} + \phi_{n,\mathbf{k}}^\dagger c_{n,\mathbf{k}\uparrow} c_{n,-\mathbf{k}\downarrow}), \] (3.14)

and following the same procedure as for the ideal Fermi gas, one can easily get

\[ \langle c_{n,\mathbf{k}\sigma}^\dagger c_{n,\mathbf{k}\sigma} \rangle = \begin{cases} 
\frac{1}{e^{\beta \epsilon_{n}(\mathbf{k})} + 1}, & \theta_{n,\mathbf{k}} = 0, \pi, \\
\frac{1}{e^{\beta' \epsilon_{n}(\mathbf{k})} + 1}, & \theta_{n,\mathbf{k}} = \pi/2, 3\pi/2,
\end{cases} \] (3.15)

where \( \theta_{n,\mathbf{k}} = |\phi_{n,\mathbf{k}}| \).

Suppose that there are, for example, two electrons per site. If the system is at zero temperature and stays in the normal phase where all \( \theta_{n,\mathbf{k}} = 0 \) or \( \pi \), the valence band, i.e., the zeroth band, is fully filled; the conduction band, i.e., the first band, and all the other higher bands are empty. This is the well-known picture for semiconductors (or insulators), which is depicted in figure 1.

Now, let us consider such a partially negative-temperature phase,

\[ \theta_{n,\mathbf{k}} = \begin{cases} 
\pi/2, \text{or } 3\pi/2, & n = 1, \\
0, \text{or } \pi, & n \neq 1.
\end{cases} \] (3.16)

If this phase is at zero temperature, the conduction band is fully filled; all the other bands are empty. This implies that the population is inverted between the valence and conduction bands, which is depicted in figure 2. As mentioned above, such a population-inversion phase is unstable; it will finally turn into the stable phase, i.e., the normal
phase, with the electrons in the conduction band hopping into the valence band and simultaneously releasing energies to the surroundings. It will make a laser if the energies are released by means of emitting photons. That is somewhat an ideal semiconductor laser: it is a ‘two-level’ system; a more realistic laser can be achieved in the so-called ‘three-level’ system,

$$\theta_{n,k} = \begin{cases} 0, \text{ or } \pi, & n = 0, \\ \pi/2, \text{ or } 3\pi/2, & \exists k \text{ for } n = 2, \\ 0, \text{ or } \pi, & \text{otherwise}, \end{cases}$$

(3.17)

where the zeroth and second bands are partially filled, and the first band is empty, which is depicted in figure 3. Here, the population is not inverted between the zeroth and second bands, i.e., the population of the second band is less than that of the zeroth band, but it is inverted between the first and second bands. This kind of ‘three-level’ semiconductor laser has been realized in experiments [33]. For this reason, we call the partially negative-
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Figure 3. Energy bands for a laser phase of a semiconductor where $\mu$ denotes the chemical potential. Here, both the valence and second bands are partially filled; the population is inverted between the second and conduction bands.

temperature phase the laser phase. Obviously, a laser phase cannot be described by the original Gibbs ensemble theory [1].

Traditionally, negative temperatures are something obscure, and it is hard to understand why they are higher or hotter than positive temperatures [34]–[36]. From the viewpoint of the extended ensemble theory, the reason is that both the negative-temperature and laser phases are unstable; they will tend, by giving up parts of their internal energy to the surroundings, towards the stable phase, namely, the positive-temperature phase. That is the microscopic interpretation of negative temperatures.

Finally, we note that the ideal Fermi gas cannot produce superconductivity because there does not exist any Cooper pair in any case of the solutions of equation (3.7),

$$\langle c_{-k\downarrow}c_{k\uparrow} \rangle = \text{Tr} (c_{-k\downarrow}c_{k\uparrow} \rho(H'(\phi,c))) = 0;$$  

(3.18)

this result is just as expected: it is completely in accordance with the BCS theory [3]–[5].

In summary, it is proved, within the framework of the extended ensemble theory, that the ideal Fermi gas cannot produce superconductivity; its normal phase is stable at any temperature. Besides, the extended ensemble theory gives a microscopic interpretation to the negative-temperature and laser phases: they originate from the same microscopic mechanism as that for phase transitions, and most importantly they are unstable.

4. Application to BCS superconductivity

4.1. The BCS mean-field theory

To study BCS superconductivity with the extended ensemble theory, one needs first to solve equation (2.4) to obtain the order parameter, and then to prove that it can satisfy the requirement of equation (2.5). Unfortunately, that is rather difficult because it is impossible to calculate $S(\phi,\beta)$ rigorously when $H(c)$ contains an interaction. As a result, we have to seek approximations. Before doing so, it is worthwhile to give a brief
survey to the self-consistent mean-field theory due to BCS [4, 5], which can be summarized as follows,

\[ H(c) \Rightarrow H_{\text{MF}}(c) = \sum_k \varepsilon(k)(c^\dagger_k c_k + c^\dagger_{-k} c_{-k}) - \Delta \sum_k (c_{-k} c_k + c^\dagger_k c^\dagger_{-k}) + \frac{1}{g} \Delta^2, \]  

Equation (4.1)

\[ \langle F(c) \rangle = \text{Tr} (F(c) \rho(H(c))) \Rightarrow \langle F(c) \rangle = \text{Tr} (F(c) \rho(H_{\text{MF}}(c))), \]  

where

\[ \Delta = g \sum_k \langle c_{-k} c_k \rangle = g \sum_k \text{Tr} (c_{-k} c_k \rho(H_{\text{MF}}(c))). \]  

Equations (4.1) and (4.3) constitute a pair of self-consistent equations to determine both the mean-field Hamiltonian \( H_{\text{MF}}(c) \) and the energy gap \( \Delta \). After \( H_{\text{MF}}(c) \) is so determined, the average of observable \( F(c) \) can be evaluated according to equation (4.2).

Obviously, if \( \Delta \neq 0 \), the mean-field Hamiltonian \( H_{\text{MF}}(c) \) is not invariant under the gauge transformation of equation (1.3), i.e., the gauge symmetry is broken with respect to \( H_{\text{MF}}(c) \). It should be noted that, as shown in equations (4.2) and (4.3), \( H_{\text{MF}}(c) \) must be used in place of \( H(c) \) when calculating statistical averages. Otherwise, \( \Delta \) becomes zero, and there is no Cooper pair and superconductivity, as has been demonstrated in equation (1.4). That is the key point of the BCS mean-field theory. This kind of mean-field theory is also widely used in studying other phase transitions and SSB, Bogoliubov theory of a weakly interacting Bose gas being a famous example [37, 38]. Nevertheless, as pointed out by Emch in section 1.1.f of [13], it contains an inescapable paradox. That is, the spectrum of the system Hamiltonian \( H_{\text{MF}}(c) \) depends on temperature, which contradicts the fact that the spectrum of an operator is an invariant property of this operator itself and should not depend on temperature. Now, for the extended ensemble theory, the normal and superconducting phases correspond, as stated in section 2, to the symmetric and asymmetric representations of the same system Hamiltonian, respectively; this excludes such a paradox absolutely.

Although the approximation of equations (4.1)–(4.3) contains the paradox, its results are astonishingly in good agreement with the experiments. Therefore, we need to search for a formally identical but essentially different approximation within the extended ensemble theory so as to interpret the superconductivity anew.

In the language of Green’s function (GF), the above approximation can be translated into the following formalism,

\[ \langle \langle c_k \mid c^\dagger_{k\downarrow} \rangle \rangle^\text{MF}_{\omega} = \frac{\omega + \varepsilon(k)}{\omega^2 - [\varepsilon^2(k) + \Delta^2]}, \]  

Equation (4.4)

\[ \langle \langle c_k \mid c_{-k\downarrow} \rangle \rangle^\text{MF}_{\omega} = \frac{\Delta}{\omega^2 - [\varepsilon^2(k) + \Delta^2]}, \]  

Equation (4.5)

\[ \Delta = -g \sum_k \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} f(\omega) \text{Im} \langle \langle c_k \mid c_{-k\downarrow} \rangle \rangle^\text{MF}_{\omega}, \]  

Equation (4.6)

where \( \langle \langle A \mid B \rangle \rangle^\text{MF}_{\omega} \) denotes the retarded Green’s function defined with respect to \( H_{\text{MF}}(c) \). Now, equations (4.5) and (4.6) constitute a pair of self-consistent equations to determine
the two complex-valued functions, $\langle \langle c_k | c_{-k} \rangle \rangle_{\omega}^{\text{MF}}$ and $\Delta$, in contrast to equations (4.1) and (4.3), where an operator is involved. Therefore, equations (4.4)–(4.6) are formally adaptable to transplanting into the extended ensemble theory. As is well known, BCS superconductivity can be explained in terms of these Green’s functions [4, 5]. We shall reestablish them within the framework of the extended ensemble theory. Of course, they must be redefined, with respect to $H'(\phi, c)$ instead of $H_{\text{MF}}(c)$.

### 4.2. Interpretation of BCS superconductivity

Now, we devote ourselves to reestablishing a formalism similar to equations (4.4)–(4.6), and interpreting the superconductivity with the extended ensemble theory.

Following equation (3.2), the entropy of a BCS superconductor can be written as

$$S(\phi, \beta) = \ln (\text{Tr} (e^{-\beta H(c)})) + \beta \sum_k \varepsilon(k)(d_{k\uparrow}^\dagger d_{k\uparrow} + d_{-k\downarrow}^\dagger d_{-k\downarrow})$$

$$- \beta g \sum_k \sum_{k'} d_{k\uparrow}^\dagger d_{-k\downarrow}^\dagger d_{-k\downarrow} d_{k\uparrow},$$

where

$$d_{k\uparrow} = e^{-iD(\phi, c)} c_{k\uparrow} e^{iD(\phi, c)},$$

$$d_{-k\downarrow} = e^{-iD(\phi, c)} c_{-k\downarrow} e^{iD(\phi, c)},$$

and

$$A(c) \equiv \text{Tr} (A(c) \rho (H(c))).$$

As in the usual mean-field approximation, we decouple the last term on the right-hand side of equation (4.7) as follows:

$$d_{k\uparrow}^\dagger d_{-k\downarrow}^\dagger d_{-k\downarrow} d_{k\uparrow} = d_{k\uparrow}^\dagger d_{-k\downarrow}^\dagger \times d_{-k\downarrow} d_{k\uparrow}.$$  (4.10)

This results in

$$S(\phi, \beta) = \ln (\text{Tr} (e^{-\beta H(c)}))$$

$$+ \beta \sum_k \varepsilon(k) \left[ \cos^2(\theta_k)(c_{k\uparrow}^\dagger c_{k\uparrow} + c_{-k\downarrow}^\dagger c_{-k\downarrow}) + \sin^2(\theta_k)(c_{k\uparrow}^\dagger c_{k\uparrow} + c_{-k\downarrow}^\dagger c_{-k\downarrow}) \right]$$

$$- \frac{1}{\beta} \beta g \sum_{k'} \sin(2\theta_{k'}) e^{i\varphi_{k'}} (c_{k'\uparrow}^\dagger c_{k'\uparrow} - c_{-k'\downarrow}^\dagger c_{-k'\downarrow})$$

$$\times \sum_k \sin(2\theta_k) e^{-i\varphi_k} (c_{k\uparrow}^\dagger c_{k\uparrow} - c_{-k\downarrow}^\dagger c_{-k\downarrow}),$$  (4.11)

where equations (4.8), (3.3), and (1.4) have been used.

Substitution of equation (4.11) into equation (2.4) gives the equations of the order parameter,

$$2\varepsilon(k) \sin(2\theta_k) + g \cos(2\theta_k) \sum_{k'} \cos(\varphi_k - \varphi_{k'}) \sin(2\theta_{k'}) (c_{k'\uparrow}^\dagger c_{k'\uparrow} - c_{-k'\downarrow}^\dagger c_{-k'\downarrow}) = 0,$$  (4.12)

$$\sin(2\theta_k) \sum_{k'} \sin(\varphi_k - \varphi_{k'}) \sin(2\theta_{k'}) (c_{k\uparrow}^\dagger c_{k\uparrow} - c_{-k\downarrow}^\dagger c_{-k\downarrow}) = 0.$$  (4.13)
They have a trivial solution,
\[ \phi = 0, \] (4.14)
and a nontrivial solution,
\[ \varphi_k = \varphi_0 = \text{constant}, \]
\[ \varepsilon(k) \sin(2\theta_k) - \Lambda \cos(2\theta_k) = 0, \] (4.15)
where
\[ \Lambda = -ie^{i\varphi_0}g \sum_k \langle c_{-k}\downarrow c_k\uparrow \rangle. \] (4.16)

The trivial solution always remains zero: it does not change with temperature. In contrast, the nontrivial one will depend on temperature: it may be zero for some temperatures, and nonzero for the others. Without loss of generality, we shall take \( \varphi_0 = \pi/2 \); the nontrivial solution is then simplified as
\[ \varepsilon(k) \sin(2\theta_k) - \Lambda \cos(2\theta_k) = 0, \] (4.17)
\[ \Lambda = g \sum_k \langle c_{-k}\downarrow c_k\uparrow \rangle; \] (4.18)
these are a pair of coupled equations to determine both \( \theta_k \) and \( \Lambda \).

If \( g = 0 \), equation (4.18) shows that \( \Lambda = 0 \); then equation (4.17) comes back to equation (3.6) for the ideal Fermi gas. Physically, the BCS Hamiltonian of equation (1.1) can describe only the weak-coupling superconductivity. For the weak-coupling superconductivity, the coupling strength \( g \) is quite small; from equations (4.17) and (4.18) it follows that \( \Lambda \) and \( \theta_k \) are also small. This makes it easy for us to make further approximations, as will be seen below.

In order to solve equations (4.17) and (4.18), one needs \( \langle c_{-k}\downarrow c_k\uparrow \rangle \); it can be obtained by the corresponding retarded Green’s function \( \langle\langle c_k\uparrow | c_{-k}\downarrow \rangle\rangle_\omega \) defined with respect to \( H'(\phi, c) \) [39]. As is well known, \( \langle\langle c_k\uparrow | c_{-k}\downarrow \rangle\rangle_\omega \) satisfies the equation of motion,
\[ \omega\langle\langle c_k\uparrow | c_{-k}\downarrow \rangle\rangle_\omega = \langle\langle c_k\uparrow | c_{-k}\downarrow \rangle\rangle - \langle\langle c_k\uparrow | [c_{-k}\downarrow, H'(\phi, c)] \rangle\rangle_\omega, \] (4.19)
where \( \{A, B\} \) denotes the anticommutator of \( A \) and \( B \). Expanding \( H'(\phi, c) \) into the power series of \( \phi \),
\[ H'(\phi, c) = H(c) + i[D(\phi, c), H(c)] + \frac{i^2}{2!} [D(\phi, c), [D(\phi, c), H(c)]] + \cdots, \] (4.20)
and substituting it into equation (4.19), we have
\[ \omega\langle\langle c_k\uparrow | c_{-k}\downarrow \rangle\rangle_\omega = \langle\langle c_k\uparrow | c_{-k}\downarrow \rangle\rangle - \langle\langle c_k\uparrow | [c_{-k}\downarrow, H(c)] \rangle\rangle_\omega 
- i\langle\langle c_k\uparrow | [c_{-k}\downarrow, [D(\phi, c), H(c)]] \rangle\rangle_\omega 
- \frac{i^2}{2!} \langle\langle c_k\uparrow | [c_{-k}\downarrow, [D(\phi, c), [D(\phi, c), H(c)]]] \rangle\rangle_\omega + \cdots. \] (4.21)
As stated above, $\phi$ is small for the weak-coupling superconductivity; it is thus rational to maintain only the zeroth-order term,

$$
\omega \langle \langle c_k | c_{-k} \rangle \rangle_\omega = -\varepsilon(k) \langle \langle c_k | c_{-k} \rangle \rangle_\omega + g \langle \langle c_k | c_{k'}^\dagger \sum_{k'} c_{-k'} c_{k'}^\dagger \rangle \rangle_\omega. \tag{4.22}
$$

With regard to the second GF on the right-hand side, we do the factorization as in equation (4.10),

$$
g \sum_{k'} \langle \langle c_{-k'}^\dagger c_{k'}^\dagger \rangle \rangle_\omega = g \sum_{k'} d_{-k'} d_{k'} = \Lambda; \tag{4.23}
$$

this leads to

$$
[\omega + \varepsilon(k)] \langle \langle c_k | c_{-k} \rangle \rangle_\omega = \Lambda \langle \langle c_k | c_{k'}^\dagger \rangle \rangle_\omega. \tag{4.24}
$$

The GF on the right-hand side can be obtained by the same procedure as for $\langle \langle c_k | c_{-k} \rangle \rangle_\omega$,

$$
[\omega - \varepsilon(k)] \langle \langle c_k | c_{k'}^\dagger \rangle \rangle_\omega = 1 + \Lambda^\dagger \langle \langle c_k | c_{-k} \rangle \rangle_\omega, \tag{4.25}
$$

where

$$
\Lambda^\dagger = g \sum_k \langle \langle c_k^\dagger c_{-k}^\dagger \rangle \rangle_\omega = \Lambda. \tag{4.26}
$$

From equations (4.24)–(4.26), it follows that

$$
\langle \langle c_k | c_{k'}^\dagger \rangle \rangle_\omega = \frac{\omega + \varepsilon(k)}{\omega^2 - [\varepsilon^2(k) + \Lambda^2]^2}, \tag{4.27}
$$

$$
\langle \langle c_k | c_{-k} \rangle \rangle_\omega = \frac{\Lambda}{\omega^2 - [\varepsilon^2(k) + \Lambda^2]^2}, \tag{4.28}
$$

$$
\Lambda = -g \sum_k \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} f(\omega) \text{Im} \langle \langle c_k | c_{-k} \rangle \rangle_\omega. \tag{4.29}
$$

They form a self-consistent mean-field solution to the Green’s functions responsible for BCS superconductivity within the framework of the extended ensemble theory. Comparing them with equations (4.4)–(4.6), one sees that the present solution is identical to the BCS solution except that the statistical average is now defined with respect to $H'(\phi, c)$. Thus far, the BCS mean-field results have been transplanted into the extended ensemble theory; the paradox has been removed.

With the help of equation (4.28), equations (4.29) and (4.17) can be simplified as

$$
\Lambda = \frac{1}{2} g \Lambda \sum_k \text{tanh} \left( \frac{1}{2} \beta \xi_k \right) \xi_k, \tag{4.30}
$$

$$
\theta_k = \begin{cases} 
\frac{1}{2} \arcsin \left( \frac{\Lambda}{\xi_k} \right), & \varepsilon(k) \geq 0, \\
-\frac{1}{2} \arcsin \left( \frac{\Lambda}{\xi_k} \right), & \varepsilon(k) < 0,
\end{cases} \tag{4.31}
$$

where

$$
\xi_k = \sqrt{\varepsilon^2(k) + \Lambda^2}. \tag{4.32}
$$

doi:10.1088/1742-5468/2006/09/P09007

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Equation (4.31) together with equation (4.30) gives the mean-field solution to \( \phi (\phi_k = i\theta_k) \), the order parameter for BCS superconductivity.

Equation (4.30) is familiar in the BCS mean-field theory [4, 5]; it has the nontrivial solution

\[
\Lambda = \begin{cases} 
0, & T \geq T_c, \\
\text{nonzero}, & T < T_c,
\end{cases}
\] (4.33)

where \( T_c \) is determined by the equation

\[
1 = \frac{1}{2} g \sum_k \tanh \left( \frac{1}{2} \beta \varepsilon(k) \right) \frac{\varepsilon(k)}{\varepsilon(k)},
\] (4.34)

with \( \beta_c = 1/k_B T_c \). From equations (4.33) and (4.31), we find

\[
\phi_k = \begin{cases} 
0, & T \geq T_c, \\
\text{nonzero}, & T < T_c.
\end{cases}
\] (4.35)

Since \( \phi \) is the order parameter of the system, equation (4.35) indicates that \( T_c \) is the transition temperature for BCS superconductivity.

Compared with equation (4.35), equation (4.33) shows that the energy gap \( \Lambda \) behaves with temperature just like an order parameter. However, this behaviour of the energy gap is not a property of itself, but derives from the property of the order parameter, as can be seen from the equation

\[
\Lambda = g \sum_k \text{Tr} \left( c_{-k1} c_{k1} \rho (H'(\phi, c)) \right) = \begin{cases} 
0, & \phi = 0, \\
\text{nonzero}, & \phi \neq 0,
\end{cases}
\] (4.36)

which demonstrates that the forming of Cooper pairs is a direct consequence of the gauge-symmetry breaking caused by the internal spontaneous field \( \phi \). In the extended ensemble theory, the order parameter is a physical quantity more fundamental than the energy gap. This picture is significantly distinct from the BCS mean-field theory where the energy gap is the most fundamental quantity that is responsible for the superconductivity.

In sum, equations (4.27), (4.28), (4.30), and (4.31) constitute a self-consistent mean-field theory for BCS superconductivity within the framework of the extended ensemble theory; its nontrivial solution reproduces the BCS mean-field results on the conventional low-\( T_c \) superconductivity.

We are now confronted with the important task to prove the stability of this nontrivial solution. By expanding the \( S(\phi, \beta) \) of equation (4.11) into a Taylor or Volterra series in the neighbourhood of the nontrivial solution \( \phi_0 \), one finds

\[
\Delta S = S(\phi, \beta) - S(\phi_0, \beta) = \delta^2 S + \delta^3 S + \delta^4 S + \cdots,
\] (4.37)

where \( \delta^n S \) represents the \( n \)th power term of the expansion of \( S(\phi, \beta) \), or the \( n \)th variation of \( S \). Specifically, the second variation \( \delta^2 S \) has the form

\[
\delta^2 S = \frac{1}{8} \beta g \Lambda^2 \sum_k \sum_{k'} \frac{\tanh \left( \frac{1}{2} \beta \xi_k \right) \tanh \left( \frac{1}{2} \beta \xi_{k'} \right)}{\xi_k} (\delta \varphi_k - \delta \varphi_{k'})^2 + 2 \beta \sum_{k_1} \xi_{k_1} \tanh \left( \frac{1}{2} \beta \xi_{k_1} \right) \\
\times (\delta \theta_{k_1})^2 + \beta \left\{ \sum_{k_2} 2 \xi_{k_2} \tanh \left( \frac{1}{2} \beta \xi_{k_2} \right) (\delta \theta_{k_2})^2 \\n- g \sum_{k_2} \sum_{k_2'} \varepsilon(k_2) \frac{\tanh \left( \frac{1}{2} \beta \xi_{k_2} \right)}{\xi_{k_2}} \varepsilon(k_2') \frac{\tanh \left( \frac{1}{2} \beta \xi_{k_2'} \right)}{\xi_{k_2'}} (\delta \theta_{k_2} \delta \theta_{k_2'}) \right\},
\] (4.38)

\text{doi:10.1088/1742-5468/2006/09/P09007}
where \( \delta \varphi_k \) and \( \delta \theta_k \) represent the variations of \( \varphi_k \) and \( \theta_k \) from the nontrivial solution \( \phi_0 \), respectively. Here, the set of \( k \) has been separated into two subsets: the subset of \( k_1 \) and the subset of \( k_2 \), where \( k_1 \) and \( k_2 \) satisfy \( \varepsilon(k_1) = 0 \) and \( \varepsilon(k_2) \neq 0 \), respectively. All the contributions from the subset of \( k_2 \) are included by the term within the curly brackets.

Let us prove that this term is definitely positive; this can be done by proving that the eigenvalues of the matrix \( M \),

\[
M_{k_2k_2'} = 2 \xi_{k_2} \tanh \left( \frac{1}{2} \beta \xi_{k_2} \right) \delta_{k_2k_2'} - g \varepsilon(k_2) \varepsilon(k_2') \frac{\tanh(\frac{1}{2} \beta \xi_{k_2}) \tanh(\frac{1}{2} \beta \xi_{k_2}')}{\xi_{k_2}}.
\]  

(4.39)

are all positive. The eigenvalue function for \( M \) is

\[
|\Omega(\lambda)| = 0,
\]  

(4.40)

where

\[
\Omega_{k_2k_2'}(\lambda) = \lambda \delta_{k_2k_2'} - M_{k_2k_2'}.
\]  

(4.41)

Observe that the second term on the right-hand side of equation (4.39) is a product of the two factors corresponding to the row \( k_2 \) and the column \( k_2' \) respectively; we can reduce equation (4.40) into

\[
|\tilde{\Omega}(\lambda)| = 0,
\]  

(4.42)

where

\[
\tilde{\Omega}_{k_2k_2'}(\lambda) = \frac{\lambda - 2 \xi_{k_2} \tanh(\frac{1}{2} \beta \xi_{k_2})}{g \varepsilon(k_2) \tanh(\frac{1}{2} \beta \xi_{k_2})/\xi_{k_2}} \delta_{k_2k_2'} + 1.
\]  

(4.43)

Obviously,

\[
\lambda = 2 \xi_{k_2} \tanh(\frac{1}{2} \beta \xi_{k_2}) > 0
\]  

(4.44)

is an eigenvalue of equation (4.42) because at least two rows \( (\pm k_2) \) of the determinant \( |\Omega(\lambda)| \) are identical. Apart from those eigenvalues, there are possibly other ones; they satisfy the equation

\[
1 = g \sum_{k_2} \frac{[\varepsilon(k_2) \tanh(\frac{1}{2} \beta \xi_{k_2})/\xi_{k_2}]^2}{2 \xi_{k_2} \tanh(\frac{1}{2} \beta \xi_{k_2}) - \lambda}.
\]  

(4.45)

To derive this equation from equation (4.42), it is sufficient to heed that every element of \( \tilde{\Omega}(\lambda) \) contains the number 1. If \( \lambda \leq 0 \), one has

\[
g \sum_{k_2} \frac{[\varepsilon(k_2) \tanh(\frac{1}{2} \beta \xi_{k_2})/\xi_{k_2}]^2}{2 \xi_{k_2} \tanh(\frac{1}{2} \beta \xi_{k_2}) - \lambda} < \frac{1}{2} g \sum_{k} \frac{\tanh(\frac{1}{2} \beta \xi_k)}{\xi_k}.
\]  

(4.46)

Equations (4.45) and (4.46) lead us to

\[
\frac{1}{2} g \sum_{k} \frac{\tanh(\frac{1}{2} \beta \xi_k)}{\xi_k} > 1.
\]  

(4.47)

This inequality contradicts the result of equation (4.30),

\[
\frac{1}{2} g \sum_{k} \frac{\tanh(\frac{1}{2} \beta \xi_k)}{\xi_k} \leq 1.
\]  

(4.48)
That is to say, any root of equation (4.45) must be greater than zero. Combination of this result with equation (4.44) demonstrates that all the eigenvalues of the matrix $M$ are definitely positive, which ends our proof for the positivity of the term within the curly brackets of equation (4.38).

This positivity implies that

$$\delta^2 S \geq 0. \quad (4.49)$$

When $\delta^2 S > 0$, we know from equation (4.37) that $\Delta S > 0$; it meets the requirement of equation (2.5). However, if $\delta^2 S = 0$, we must generally examine $\delta^3 S$, $\delta^4 S$, or even higher variations of $S$ to check whether $\Delta S \geq 0$, which is obviously complicated to handle. Fortunately, we need not do that in the case considered now. When $\delta^2 S = 0$, equation (4.38) shows that

$$\delta \theta_{k_2} = 0, \quad \text{if } T \geq T_c; \quad \text{and} \quad \begin{cases} 
\delta \varphi_k = \delta \varphi_{k'} \\
\delta \theta_{k_1} = 0 & \text{if } T < T_c. \\
\delta \theta_{k_2} = 0,
\end{cases} \quad (4.50)$$

With them, one can easily verify that $S(\phi, \beta) = S(\phi_0, \beta)$. Namely, $\Delta S = 0$ if $\delta^2 S = 0$.

To sum up, $\Delta S > 0$ if $\delta^2 S > 0$, and $\Delta S = 0$ if $\delta^2 S = 0$. Since $\delta^2 S \geq 0$, we conclude that the requirement $\Delta S \geq 0$ is satisfied; the nontrivial solution is stable.

As regards the trivial solution, $\phi = 0$ ($\Lambda = 0$), it is identical to the nontrivial one when $T \geq T_c$, and thus is stable at $T \geq T_c$. If $T < T_c$, we find

$$\delta^2 S = \beta \left\{ \sum_{k_2} 2\varepsilon(k_2) \tanh \left( \frac{1}{2} \beta \varepsilon(k_2) \right) (\delta \theta_{k_2})^2 \\
- g \sum_{k_2} \sum_{k'_2} \tanh \left( \frac{1}{2} \beta \varepsilon(k_2) \right) \tanh \left( \frac{1}{2} \beta \varepsilon(k'_2) \right) \delta \theta_{k_2} \delta \theta_{k'_2} \right\}. \quad (4.51)$$

Accordingly, it has positive eigenvalues,

$$\lambda = 2\varepsilon(k_2) \tanh \left( \frac{1}{2} \beta \varepsilon(k_2) \right) > 0. \quad (4.52)$$

In addition, we also have

$$1 = g \sum_{k_2} \frac{\left[ \tanh \left( \frac{1}{2} \beta \varepsilon(k_2) \right) \right]^2}{2\varepsilon(k_2) \tanh \left( \frac{1}{2} \beta \varepsilon(k_2) \right) - \lambda}. \quad (4.53)$$

In contrast to equation (4.45), this equation has a negative root of $\lambda$ when $T < T_c$. To see it clearly, let us consider, for instance, the zero temperature case,

$$1 = 2g \sum_{\varepsilon(k)>0} \frac{1}{2\varepsilon(k) - \lambda} = 2g\mathcal{N}(0) \int_0^{\hbar \omega_D} d\varepsilon \frac{1}{2\varepsilon - \lambda}, \quad (4.54)$$

where, as usual, $\mathcal{N}(0)$ denotes the density of states at the Fermi level, and $\omega_D$ the Debye frequency. Apparently, it has the solution

$$\lambda = \frac{2\hbar \omega_D}{\exp(1/g\mathcal{N}(0)) - 1} < 0. \quad (4.55)$$

doi:10.1088/1742-5468/2006/09/P09007
The existence of both positive and negative eigenvalues implies that the trivial solution is a saddle point at \( T < T_c \). Therefore, the term within the curly brackets of equation (4.51) is indefinite; that is, it can change in sign. As a consequence, the trivial solution, or rather the normal phase, is unstable at \( T < T_c \). That is just the Cooper instability [3]–[5].

Of the two solutions, the nontrivial is the only one that is stable within the whole temperature range.

With the nontrivial solution obtained, other physical quantities can be easily expressed and calculated in terms of the two Green’s functions \( \langle c_{k\uparrow}^\dagger c_{k\uparrow} \rangle_\omega \) and \( \langle (c_{k\uparrow}c_{-k\downarrow})_\omega \rangle \), as was done in [5, 40] and [41], with the results unchanged and the same as the BCS theory.

So far, BCS superconductivity has been interpreted within the extended ensemble theory. In this interpretation, the order parameter for BCS superconductivity evolves with temperature according to the principle of least entropy. At high temperatures (\( T \geq T_c \)), it is zero and stable; the system Hamiltonian realizes the representation with perfect gauge symmetry, and the resulting phase is normal and disordered. As the temperature decreases and goes below the critical temperature (\( T < T_c \)), the zero solution becomes unstable; instead, there arises a new stable solution of the order parameter: it is nonzero. At the same time, the system Hamiltonian transforms into a new representation with gauge symmetry broken: the electrons are hence formed into Cooper pairs, and the resulting phase becomes superconducting. Thus the extended ensemble theory answers why, when and how the electrons can coagulate to form Cooper pairs and superconductivity, the problem posed by Born and Fuchs [22].

Lastly, it should be noted that the BCS and Landau theories are unified into a single formalism within the framework of the extended ensemble theory.

5. Bose–Einstein condensation

After the discussion of BCS superconductivity, we proceed now to study Bose–Einstein condensation (BEC). We shall concentrate on three systems: the ideal Bose gas, the photon gas in a black body, and the ideal phonon gas in a solid body. They are the most important cases of Bose systems: the first is a system with the conservation of particles, but the other two are not; the second belongs to gauge fields, whereas the third does not. In addition, we shall also discuss the quantization of the Dirac field from a standpoint of the extended ensemble theory.

5.1. The ideal Bose gas

Let us begin with the ideal Bose gas. Its Hamiltonian reads as follows:

\[
H(b) = \sum_k (\epsilon_k - \mu) b_k^\dagger b_k, \tag{5.1}
\]

where \( b_k \) (\( b_k^\dagger \)) is the annihilation (creation) operator for the bosons with a momentum \( \hbar k \), \( \epsilon_k = \hbar^2 k^2 / (2m) \) the single-particle energy, and \( \mu \) the chemical potential. This Hamiltonian is gauge invariant,

\[
G(\vartheta, b)H(b)G^\dagger(\vartheta, b) = H(b), \tag{5.2}
\]
where

\[ G(\vartheta, b) = e^{-i\vartheta \sum_k b_k^\dagger b_k}, \quad \vartheta \in [0, 2\pi). \]  

(5.3)

The invariance has an important consequence:

\[ \langle b_k \rangle = \text{Tr} (b_k \rho(H(b))) = 0. \]  

(5.4)

This signifies that the condensation amplitude will be zero forever if the gauge symmetry does not break down.

In order to examine whether the gauge symmetry can break down spontaneously or not, one needs, following the hypotheses in section 2, to consider the phase-transition operator,

\[ D(\eta, b) = \sum_k (\eta_k^\dagger b_k + \eta_k b_k^\dagger), \]  

(5.5)

where the internal field \( \eta \) is the order parameter for BEC. The reason for introducing equation (5.5) can be seen from comparing equations (5.4) and (5.5) with equations (1.4) and (2.2) respectively.

We shall consider first the finite volume case where \( V \) and \( N \) are both finite, and then the thermodynamic limit case where \( V \to +\infty \), and \( N \to +\infty \), but \( N/V \) is finite. As will be seen, the two cases are significantly different.

5.1.1. The finite volume case. In this case, the wavevector \( k \) is discrete. The entropy of the system can be written as

\[ S(\eta, \beta) = S(0, \beta) + \beta \sum_k (\epsilon_k - \mu) \eta_k^\dagger \eta_k, \]  

(5.6)

where

\[ S(0, \beta) = -\text{Tr} (\ln (\rho(H(b))) \rho(H(b))) \]  

(5.7)

is independent of the order parameter \( \eta \). According to equations (2.4) and (2.5), we have

\[ \frac{\partial S}{\partial \eta_k} = 0, \]  

(5.8)

\[ \Delta S = \beta \sum_k (\epsilon_k - \mu) \delta \eta_k^\dagger \delta \eta_k \geq 0, \]  

(5.9)

where \( \delta \eta_k \) represents the variation of \( \eta_k \) from the solution given by equation (5.8). Equation (5.9) shows that the chemical potential \( \mu \) must satisfy the following condition:

\[ \mu \leq \epsilon_k. \]  

(5.10)

As \( \epsilon_k \geq 0 \), this condition is equivalent to

\[ \mu \leq 0. \]  

(5.11)

This inequality is the physical condition for the stability of the system.

In combination with equations (5.6), (5.8) gives us the equation of the order parameter,

\[ (\epsilon_k - \mu) \eta_k = 0. \]  

(5.12)
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It has two solutions: the trivial one,
\[ \eta_k = 0, \]
and the nontrivial one,
\[ \eta_k = \eta_0 \delta_{k,0}, \quad \text{only if } \mu = 0. \] (5.14)

For the nontrivial solution, \( \mu = 0 \), it causes a contradiction,
\[ \eta_0^+ \eta_0 = N - \sum_k \text{Tr} \left( b_k^\dagger b_k \rho(H(b)) \right) \]
\[ = N - \sum_k \frac{1}{\epsilon_k - \mu}, \] (5.15)
where the left-hand side cannot be negative, but the right-hand side is negative because the term of \( k = 0 \) is infinite. Therefore, the nontrivial solution must be discarded.

With regard to the trivial solution, it corresponds to the normal phase of the system. It does not cause any contradiction,
\[ N = \sum_k \text{Tr} \left( b_k^\dagger b_k \rho(H(b)) \right) = \sum_k \frac{1}{e^{\beta \epsilon_k} - 1}; \] (5.16)
this equation can be satisfied at any temperature. In fact, it is just the equation for the chemical potential \( \mu \); its solution will give \( \mu = \mu(T) \). Because \( N \) is finite, \( \mu \) will be less than zero irrespective of temperature, i.e.,
\[ \mu(T) < 0, \quad \text{for } T > 0. \] (5.17)
This implies that the normal phase of the system is always stable,
\[ \Delta S > 0. \] (5.18)
This proves that there is no phase transition in the finite volume case; the system will stay in its normal phase forever.

5.1.2. The thermodynamic limit case. In this case, \( V \to +\infty \), we should use the density of entropy instead of the entropy itself,
\[ s(\eta, \beta) = \lim_{V \to +\infty} \frac{S(\eta, \beta)}{V} \]
\[ = s(0, \beta) + \beta \lim_{V \to +\infty} \frac{1}{V} \sum_k (\epsilon_k - \mu) \eta_k^\dagger \eta_k; \] (5.19)
where
\[ s(0, \beta) = - \lim_{V \to +\infty} \frac{1}{V} \text{Tr} \left( \ln \left( \rho(H(b)) \right) \rho(H(b)) \right) \] (5.20)
is a term irrelevant to \( \eta \). The limit \( V \to +\infty \) can be achieved as follows.

As usual, suppose that the system is box normalized, i.e.,
\[ k_{x(y,z)} = n_{x(y,z)} \frac{2\pi}{l_{x(y,z)}}, \quad n_{x(y,z)} \in \mathbb{Z}, \] (5.21)
where $\mathbb{Z}$ denotes the set of integers, and $l_x$, $l_y$, and $l_z$ the dimensions of the box along the $x$, $y$ and $z$ directions respectively ($V = l_x l_y l_z$). As is well known, each $\mathbf{k}$ corresponds to an eigenfunction; all the eigenfunctions constitute a Hilbert space. Here, the Hilbert space is a complete space of integrable functions, with the inner product defined as a Lebesgue integral. It should be pointed out that the inner product must be defined as a Lebesgue rather than Riemann integral because the former can ensure the completeness of an integrable function space whereas the latter cannot [42]. This implies that all the problems relevant to a Hilbert space of integrable functions must be treated with Lebesgue theory. On the other hand, Lebesgue measure and integration is itself the mathematical foundation of probability theory [43,44] and statistical physics [11]. We shall therefore perform the thermodynamic limit according to the Lebesgue theory of integration.

Formally, Lebesgue integration includes both the sum over discrete numbers and the integral on a continuous region. When $V$ is finite, a sum over $\mathbf{k}$ is a Lebesgue integral of discrete form. It will transform into a Lebesgue integral of continuous form as $V \to +\infty$.

To show the transformation, let us consider, for example, the sum over $\mathbf{k}$ in equation (5.19). In the first place, we write it into an explicit form of a Lebesgue integral,

$$
\frac{1}{V} \sum_k (\epsilon_k - \mu) \eta_k^\dagger \eta_k = \frac{1}{(2\pi)^3} \sum_k (\epsilon_k - \mu) \eta_k^\dagger \eta_k m(A_k \cap \mathbb{R}^3) = \frac{1}{(2\pi)^3} \int_E h(\mathbf{p}) \, d\mathbf{p},
$$

(5.22)

where

$$
\mathbb{R}^3 = (-\infty, +\infty) \times (-\infty, +\infty) \times (-\infty, +\infty),
$$

(5.23)

$$
m(A_k \cap \mathbb{R}^3) = \frac{(2\pi)^3}{V},
$$

(5.24)

$$
A_k = \left[ k_x, k_x + \frac{2\pi}{l_x} \right) \times \left[ k_y, k_y + \frac{2\pi}{l_y} \right) \times \left[ k_z, k_z + \frac{2\pi}{l_z} \right),
$$

(5.25)

$$
h(\mathbf{p}) = \sum_k (\epsilon_k - \mu) \eta_k^\dagger \eta_k \chi_{A_k}(\mathbf{p}),
$$

(5.26)

$$
\chi_{A_k}(\mathbf{p}) = \begin{cases} 1, & \mathbf{p} \in A_k, \\ 0, & \mathbf{p} \not\in A_k. \end{cases}
$$

(5.27)

As usual, $\chi_{A_k}(\mathbf{p})$ represents the characteristic function of the measurable set $A_k$, and $m(A_k \cap \mathbb{R}^3)$ the Lebesgue measure of the set $A_k$. From equations (5.25)–(5.27), it follows that

$$
\lim_{V \to +\infty} h(\mathbf{p}) = (\epsilon_\mathbf{p} - \mu) \eta_\mathbf{p}^\dagger \eta_\mathbf{p} \\
\equiv [\epsilon(\mathbf{p}) - \mu] \eta^\dagger(\mathbf{p}) \eta(\mathbf{p}).
$$

(5.28)

Now, in the second place, let us take the thermodynamic limit on both sides of equation (5.22),

$$
\lim_{V \to +\infty} \frac{1}{V} \sum_k (\epsilon_k - \mu) \eta_k^\dagger \eta_k = \lim_{V \to +\infty} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} h(\mathbf{p}) \, d\mathbf{p} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \lim_{V \to +\infty} h(\mathbf{p}) \, d\mathbf{p}
$$

$$
= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} [\epsilon(\mathbf{k}) - \mu] \eta^\dagger(\mathbf{k}) \eta(\mathbf{k}) \, d\mathbf{k}.
$$

(5.29)
In such a natural way, a discrete sum over \( k \) will transform into a continuous Lebesgue integral in the thermodynamic limit.

With the help of the above equation, one arrives at

\[
\epsilon(k) - \mu \eta(k) = 0,
\]

\[
\Delta s = \beta \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} [\epsilon(k) - \mu] \delta \eta^\dagger(k) \delta \eta(k) dk \geq 0.
\]

The second equation means that the chemical potential must be less than or equal to zero,

\[
\mu \leq 0;
\]

it is the condition for the stability of the system. The first equation is equivalent to

\[
\epsilon(k) - \mu \eta^\dagger(k) \eta(k) = 0,
\]

which can be easily verified with respect to the two cases: \( \eta^\dagger(k) = 0 \) and \( \eta^\dagger(k) \neq 0 \).

Equation (5.33) has two solutions: the trivial one,

\[
\eta(k) = 0,
\]

and the nontrivial one,

\[
\eta(k) = \xi \sqrt{\delta(k)}, \quad \text{only if } \mu = 0,
\]

where \( \xi \) is a complex which does not depend on \( k \), and \( \delta(k) \) the Dirac \( \delta \) function.

For the trivial solution, the system is in its normal phase; this phase can exist only at high temperatures, which can be easily deduced from the equation of chemical potential,

\[
n \equiv \lim_{V \to +\infty} \frac{N}{V} = \lim_{V \to +\infty} \frac{1}{V} \sum_k \text{Tr} \left( b_k^\dagger b_k \rho(H(b)) \right)
\]

\[
= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{1}{e^{\beta(\epsilon(k) - \mu)} - 1} dk
\]

\[
= \frac{(2m)^{3/2}}{4\pi^2 h^3} \int_{0^+}^{+\infty} d\epsilon \frac{\epsilon^{1/2}}{e^{\beta \epsilon} - 1},
\]

where we have reduced the Lebesgue integral into an improper Riemann integral at the end. Because, as shown by equation (5.32), \( \mu \) must be less than or equal to zero, the above equation cannot hold if \( T < T_c \), where \( T_c \) is determined by

\[
n = \frac{(2m)^{3/2}}{4\pi^2 h^3} \int_{0^+}^{+\infty} d\epsilon \frac{\epsilon^{1/2}}{e^{\beta \epsilon} - 1}.
\]

As is well known, this gives

\[
T_c = \frac{2\pi \hbar^2}{mk_B} \left( \frac{n}{\zeta(3/2)} \right)^{2/3},
\]

where \( \zeta(x) \) denotes the Riemann zeta function.
For the nontrivial solution, $\mu$ must be zero, and the order parameter is determined by

$$n = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \eta^\dagger(k)\eta(k)\,dk + \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{1}{e^{\beta\epsilon(k)} - 1}\,dk$$

$$= \frac{1}{(2\pi)^3} \xi^\dagger\xi + \frac{(2m)^{3/2}}{4\pi^2\hbar^3} \int_0^{+\infty} d\epsilon \frac{\epsilon^{1/2}}{e^{\beta\epsilon} - 1},$$

(5.39)

where we have used the fact that the contribution from the state of $k = 0$ is zero when reducing the Lebesgue integral into the improper Riemann integral at the end. Because $\xi^\dagger\xi \geq 0$, the above equation cannot hold if $T > T_c$.

From those discussions, it follows that

$$\eta = \begin{cases} \text{zero}, & T \geq T_c, \\ \text{nonzero}, & T < T_c. \end{cases}$$

(5.40)

That is to say, a phase transition will happen at $T = T_c$. Because $\Delta s \geq 0$ when $\mu \leq 0$, the normal phase ($\eta = 0$) exists and is stable at $T \geq T_c$; the ordered phase ($\eta \neq 0$) exists and is stable at $T < T_c$. Here, we note that it is a natural consequence of the extended ensemble theory that the chemical potential of the ideal Bose gas is fixed at zero ($\mu = 0$) in the ordered phase ($T < T_c$), in contrast to Einstein's treatment where it is fixed by physical insight [45, 46].

Obviously, the above results are the same as the BEC given by Einstein [45, 46] if $\xi^\dagger\xi/(2\pi)^3$ were regarded as the density of the bosons condensed onto the state of $k = 0$. Therefore, the transition happening at $T = T_c$ must be identified physically as Bose–Einstein condensation. It should be pointed out that, generally, the quantity $\xi^\dagger\xi/(2\pi)^3$ cannot be interpreted as the density of condensed bosons, as will be clarified in section 7.1.

So far, we have presented a new description of the Bose–Einstein condensation of the ideal Bose gas. In comparison with Einstein’s description [45, 46], we now describe the BEC with two new conceptions: spontaneous symmetry breaking and Lebesgue integration. Within this new description, the BEC happens simultaneously with the spontaneous breaking of the gauge symmetry; the integration is defined and performed in a Lebesgue way. That is fundamentally different from Einstein’s description [45, 46], where the BEC happens with no symmetry breaking, and the integration is done in a Riemann way.

Here, it is worth emphasizing the important role played by Lebesgue integration in the study of the BEC of the ideal Bose gas. As has been seen, there arises the Bose distribution function,

$$f(\epsilon(k)) = \frac{1}{e^{\beta\epsilon(k)} - 1},$$

(5.41)

which is unbounded above on the set $E$. Because the integrand of a Riemann integral must be bounded everywhere, such a function is not Riemann integrable and cannot be handled with Riemann integration. Fortunately, that causes no trouble. As pointed out above, it is, in fact, unnecessary for us to handle the Bose distribution function with Riemann integration; what really confronts us in statistical physics is Lebesgue rather than Riemann integration. Lebesgue integration permits more general functions as integrands,
and treats bounded and unbounded functions on an equal footing. In the sense of Lebesgue integration, the Bose distribution function is integrable, which can be shown as follows:

$$
\lim_{V \to +\infty} \frac{1}{V} \sum_{k} \frac{1}{e^{\beta k} - 1} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{1}{e^{\beta k} - 1} \, dk
$$

$$
= \frac{1}{(2\pi)^3} \int_{E_0} \frac{1}{e^{\beta k} - 1} \, dk + \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3 \setminus E_0} \frac{1}{e^{\beta k} - 1} \, dk
$$

$$
= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3 \setminus E_0} \frac{1}{e^{\beta k} - 1} \, dk = \frac{(2m)^{3/2}}{4\pi^2\hbar^3} \int_{0^+}^{+\infty} \frac{dc}{e^{\epsilon/2}} e^{\epsilon/2} - 1,
$$

(5.42)

where the set $E_0 \equiv \{k = 0\}$ includes one point only. $E_0$ is a null set, i.e., its measure is zero; thus, the integral on it vanishes. The remaining part, i.e., the integral on $\mathbb{R}^3 \setminus E_0$, reduces finally into an improper Riemann integral. As is well known, the integral on a null set always vanishes irrespective of the integrand values on this set, even if they are infinite. Thereby, the integral on any single state equals zero; the ground state $(k = 0)$ is not more advantageous than the other states $(k \neq 0)$. In other words, the singularity of $f(\epsilon(k))$ on the point $k = 0$ has no special meaning, both in mathematics and in physics.

This aspect makes the present treatment quite distinct from that of Einstein, where the integration is handled in a Riemann way, with a special treatment given to the ground state of $k = 0$. Intuitively, Einstein thought that the bosons would gather in the ground state if $T < T_c$, and thus the contribution from this state is nonzero $[45, 46]$; that is,

$$
n = \lim_{V \to +\infty} \frac{1}{V} \sum_{k} \frac{1}{e^{\beta k} - 1} = n_0 + \frac{(2m)^{3/2}}{4\pi^2\hbar^3} \int_{0^+}^{+\infty} \frac{dc}{e^{\epsilon/2}} e^{\epsilon/2} - 1,
$$

(5.43)

where $n_0 > 0$ is the particle density gathering in the ground state. Comparing equations (5.39), (5.42) and (5.43) shows more clearly the difference between the present treatment and Einstein’s. From this difference it follows that the quantity $\xi^3\xi/(2\pi)^3$ need not be interpreted as the density of the bosons condensed onto the state of $k = 0$. In fact, equation (5.39) is physically just an equation of the order parameter. Here, it should be noted that the Bogoliubov theory of a weakly imperfect Bose gas $[37, 38]$ is based on equation (5.43) rather than equation (5.42). Finally, why did Einstein not use Lebesgue integration? There is a historical reason: in 1925, when Einstein $[45, 46]$ studied BEC, Lebesgue integration had not yet been introduced to probability theory by Kolmogorov, who did it in 1933 $[43]$.

Also, it is significant to compare the two Lebesgue integrals represented in equations (5.15) and (5.39): both integrands are unbounded on $\mathbb{R}^3$; however, the former is infinite on a set with a nonzero measure $(m(A_{k=0} \cap \mathbb{R}^3) = (2\pi)^3 / V)$, and the latter is finite almost everywhere, or infinite just on a null set $(m(E_0 \cap \mathbb{R}^3) = 0)$. This difference leads to the result that the nontrivial solution must be discarded in the finite volume case whereas it has physical sense in the thermodynamic limit. In a word, the ideal Bose gas can produce BEC in the thermodynamic limit, but it cannot in the finite volume case. That is a rigorous conclusion deduced from the extended ensemble theory.

As another instance, the ideal Bose gas shows unambiguously that Gibbs ensemble theory needs some kind of extension. Otherwise, the conservation of particles will be broken when $T < T_c$, as can be seen by comparing equations (5.42) and (5.43).

doi:10.1088/1742-5468/2006/09/P09007
As the one and only quantum phase transition that can be solved exactly, the BEC of the ideal Bose gas demonstrates that the extended ensemble theory postulated in section 2 is feasible in physics for us to describe phase transitions.

Lastly, we would like to stress that the condition of equation (5.32), i.e., \( \mu \leq 0 \), is not a mathematical limit but just a physical requirement. Like the case of \( \mu \leq 0 \), the extended ensemble theory is also well defined mathematically for \( \mu > 0 \), as is shown in appendix A. Removing the limitation on the chemical potential is physically reasonable; it enables the conservation of particles to be handled freely, and makes it easy to describe the BEC in the interacting Bose gas, as can be seen in section 7.1.

Remark 1. The ideal Bose gas is a touchstone for the theory of phase transitions because it is the only one of the many-body systems that can show a quantum phase transition and can be solved rigorously. Any theory of phase transitions must be examined by the ideal Bose gas. It cannot be accepted in physics if it cannot give a rigorous solution to the ideal Bose gas; and it can be further applied to the interacting Bose gas only after it has given a rigorous solution to the ideal Bose gas.

Remark 2. In 1926, Uhlenbeck [47] raised an objection to Einstein’s viewpoint on the condensation: he argued that the ideal Bose gas cannot produce BEC if the volume of the system remains finite. This objection caused an exciting debate during the van der Waals Century Conference in November 1937 [48]. Evidently, the present theory has given the exact answer to the debate: Uhlenbeck and Einstein are both right, which is also in accordance with the agreement reached finally in the conference.

Remark 3. In the momentum space used here, the condensed phase is shown to be homogeneous. In section 7.1, using real space, we shall prove further that the condensed phase can only be homogeneous. There cannot exist any supercurrent or quantized vortex in the ideal Bose gas.

Remark 4. The rigorous solution for the ideal Bose gas shows that the extended ensemble theory holds in the critical region.

5.2. The photon gas in a black body

For the photon gas in a black body, its Hamiltonian reads

\[
H(a) = \sum_{k \nu} \omega_k \left( a_{k \nu}^\dagger a_{k \nu} + \frac{1}{2} \right),
\]

(5.44)

where Coulomb gauge is used, \( a_{k \nu} \) (\( a_{k \nu}^\dagger \)) is the destruction (construction) operator for the photons with momentum \( k \) and polarization \( \nu \), and \( \omega_k = \hbar c k \) represents the photon energy with \( c \) the speed of light.

Analogous to the ideal Bose gas, this system has the phase-transition operator,

\[
D(\xi, a) = \sum_{k \nu} (\xi_{k \nu}^\dagger a_{k \nu} + \xi_{k \nu} a_{k \nu}^\dagger),
\]

(5.45)

where \( \xi \) is the order parameter for BEC.
From $H(a)$ and $D(\xi, a)$, it follows that
\[ \omega_k \xi_{k\nu} = 0, \tag{5.46} \]
\[ \Delta S = \beta \sum_{k, \sigma} \omega_k \delta \xi_{k, \sigma}^{\dagger} \delta \xi_{k, \sigma}. \tag{5.47} \]
The first is the equation of motion of the order parameter; it has the solution
\[ \xi_{k\nu} = \lambda_{\nu} \delta_{k, 0}, \tag{5.48} \]
where $\lambda_{\nu}$ is a complex constant which does not depend on $T$. Owing to the fact that $\omega_k \geq 0$, this solution is stable,
\[ \Delta S \geq 0. \tag{5.49} \]
To determine $\lambda_{\nu}$, it is sufficient to consider the initial state at $\beta = 0$ ($T \to +\infty$). Physically, any system must stay in its disordered phase at $\beta = 0$. Therefore, $\lambda_{\nu}$ must be zero at $\beta = 0$. Since $\lambda_{\nu}$ does not depend on $\beta$, it is always zero. That is to say,
\[ \xi(\beta = 0), \quad \text{for } \beta \geq 0. \tag{5.50} \]
This equation shows that the photon gas in a black body cannot produce BEC, and must always stay in its normal phase. Equation (5.49) demonstrates that the normal phase is stable. This result is also valid for the thermodynamic limit case.

In short, there cannot arise BEC in the photon gas in a black body: the system stays in its normal phase forever, and Planck’s radiation law holds at any temperature. Obviously, this conclusion agrees completely with the experiment.

5.3. The ideal phonon gas in a solid body

As the third system, let us consider the ideal phonon gas in a solid body, whose Hamiltonian reads
\[ H(d) = \sum_{k, \sigma} \omega_{k\sigma} \left( d_{k\sigma}^\dagger d_{k\sigma} + \frac{1}{2} \right), \tag{5.51} \]
where $d_{k\sigma}$ ($d_{k\sigma}^\dagger$) is the destruction (construction) operator for the phonons with momentum $k$ and polarization $\sigma$, and $\omega_{k\sigma} = \hbar c_{\sigma} k$ represents the phonon energy with $c_{\sigma}$ the velocity of sound.

By comparing equation (5.51) with equation (5.44), one concludes at once that the ideal phonon gas in a solid body cannot produce BEC either, and must also stay in its normal phase forever.

5.4. Quantization of Dirac field

Finally, let us consider the quantization of the Dirac field from the standpoint of the extended ensemble theory hypothesized in section 2. If one quantizes the Dirac field using Bose–Einstein statistics, one has the following Hamiltonian [49]:
\[ H(b; d) = \sum_{p, \sigma} \omega_p \left( b_{p, \sigma}^\dagger b_{p, \sigma} - d_{p, \sigma}^\dagger d_{p, \sigma} \right), \tag{5.52} \]

\[ \text{doi:10.1088/1742-5468/2006/09/P09007} \]
where \( \mathbf{p} \) and \( \sigma \) denote momentum and spin, respectively; \( b_{\mathbf{p},\sigma} \) (\( b_{\mathbf{p},\sigma}^\dagger \)) and \( d_{\mathbf{p},\sigma} \) (\( d_{\mathbf{p},\sigma}^\dagger \)) are bosonic destruction (construction) operators; and
\[
\omega(\mathbf{p}) = \sqrt{(c\mathbf{p})^2 + (mc^2)^2}
\] (5.53)
with \( m \) and \( c \) being the electron mass and the speed of light, respectively.

Evidently, this system has the phase-transition operator,
\[
D(\eta, b; \xi, d) = \sum_{\mathbf{p},\sigma} (\eta_{\mathbf{p},\sigma} b_{\mathbf{p},\sigma} + \xi_{\mathbf{p},\sigma}^\dagger d_{\mathbf{p},\sigma} + \eta_{\mathbf{p},\sigma}^\dagger b_{\mathbf{p},\sigma}^\dagger + \xi_{\mathbf{p},\sigma} d_{\mathbf{p},\sigma}^\dagger),
\] (5.54)
where \( \eta \) and \( \xi \) are the order parameters for BEC.

Equations (2.4) and (2.5) imply that
\[
\eta_{\mathbf{p},\sigma} = 0, \quad \xi_{\mathbf{p},\sigma} = 0,
\] (5.55, 5.56)
\[
\Delta S = \beta \sum_{\mathbf{p},\sigma} \omega_\mathbf{p} (\delta \eta_{\mathbf{p},\sigma}^\dagger \delta \eta_{\mathbf{p},\sigma} - \delta \xi_{\mathbf{p},\sigma}^\dagger \delta \xi_{\mathbf{p},\sigma}).
\] (5.57)

Equations (5.55) and (5.56) show that the system should always stay in its normal phase, but equation (5.57) demonstrates that this normal phase corresponds to a saddle point, and is thus unstable. Therefore, if the Dirac field were quantized using Bose–Einstein statistics, the system would be unstable and collapse. In other words, it is not admissible to quantize the Dirac field using Bose–Einstein statistics. This conclusion is in accordance with the spin-statistics theorem in quantum field theory [49].

On the other hand, if the Dirac field is quantized using Fermi–Dirac statistics, its Hamiltonian will read as follows [49]:
\[
H(b; d) = \sum_{\mathbf{p},\sigma} \omega_\mathbf{p} (b_{\mathbf{p},\sigma}^\dagger b_{\mathbf{p},\sigma} + d_{\mathbf{p},\sigma}^\dagger d_{\mathbf{p},\sigma});
\] (5.58)
now \( b_{\mathbf{p},\sigma} \) (\( b_{\mathbf{p},\sigma}^\dagger \)) and \( d_{\mathbf{p},\sigma} \) (\( d_{\mathbf{p},\sigma}^\dagger \)) are fermionic destruction (construction) operators for electrons and positrons. According to section 2, its phase-transition operator is
\[
D(\phi, b; \zeta, d) = \sum_k [(\phi_k b_{-k,1} b_{k,1}^\dagger + \phi_k^\dagger b_{-k,1}^\dagger b_{k,1}) + (\zeta_k d_{-k,1} d_{k,1}^\dagger + \zeta_k^\dagger d_{-k,1}^\dagger d_{k,1})],
\] (5.59)
where \( \phi \) and \( \zeta \) are order parameters. Following the arguments of section 3, one recognizes immediately that the system is always stable in its normal phase. This holds even in the original representation of the Hamiltonian [49],
\[
H(c) = \sum_\mathbf{p} \omega_\mathbf{p} \left( \sum_{s=1}^{2} c_{\mathbf{p},s}^\dagger c_{\mathbf{p},s} - \sum_{s=3}^{4} c_{\mathbf{p},s}^\dagger c_{\mathbf{p},s} \right),
\] (5.60)
where
\[
c_{\mathbf{p},s} = \begin{cases} b_{\mathbf{p},s}, & s = 1, 2, \\ d_{\mathbf{p},s-2}^\dagger, & s = 3, 4, \end{cases}
\] (5.61)
\[
D(\phi, \zeta, c) = \sum_k [(\phi_k c_{-k,2} c_{k,1} + \phi_k^\dagger c_{-k,1}^\dagger c_{k,2}) + (\zeta_k c_{-k,4} c_{k,3} + \zeta_k^\dagger c_{-k,3}^\dagger c_{k,4})].
\] (5.62)
In contrast to the electron–positron representation of equation (5.58), a minus sign appears in the original representation of equation (5.60), but it cannot influence the stability of the system. Anyway, there is no problem when the Dirac field is quantized using Fermi–Dirac statistics.

In this section, the systems concerned are free boson fields; they can all be solved rigorously. We shall proceed to the interacting systems in section 7. Generally, they cannot be solved rigorously; approximations are needed.

6. Physical origination for phase transitions

Before proceeding forward to the interacting Bose systems, it is worth doing research into the physical origination for phase transitions.

Again, let us take BCS superconductivity as an instance. According to equation (2.3), the statistical average of a one-body operator can be reformulated as

$$\int \text{d}r \langle \psi^\dagger(r) f(r) \psi(r) \rangle = \int \text{d}r \text{Tr} \left( \tilde{\psi}^\dagger(r) f(r) \tilde{\psi}(r) \rho(H(c)) \right)$$

$$= \int \text{d}r \frac{\tilde{\psi}^\dagger(r) f(r) \tilde{\psi}(r)}{\psi^\dagger(r) f(r) \psi(r)}, \quad (6.1)$$

where $\psi(r)$ is the electron field, $f(r)$ stands for the one-body operator in Schrödinger picture, and

$$\tilde{\psi}(r) = e^{-iD(\phi,c)} \psi(r) e^{iD(\phi,c)}. \quad (6.2)$$

After the phase transition ($\phi \neq 0$), the electron field $\tilde{\psi}(r)$ is separated into two fields,

$$\tilde{\psi}(r) = \psi(r) + \varphi(r), \quad (6.3)$$

where

$$\varphi(r) = e^{-iD(\phi,c)} \psi(r) e^{iD(\phi,c)} - \psi(r). \quad (6.4)$$

Substituting equation (6.3) into equation (6.1), we obtain

$$\int \text{d}r \langle \psi^\dagger(r) f(r) \psi(r) \rangle = \int \text{d}r [\psi^\dagger(r) + \varphi^\dagger(r)] [f(r) \psi(r) + \varphi(r)]. \quad (6.5)$$

The right-hand side shows that there exists interference; as usual, it is described by the cross terms,

$$\overline{\psi^\dagger(r) f(r) \varphi(r)} + \overline{\varphi^\dagger(r) f(r) \psi(r)}. \quad (6.6)$$

In terminology of quantum optics, it represents the single-particle interference. This single-particle interference will vanish if the system goes into the normal phase where $\varphi(r) = 0$. A special case is the interference appearing in the particle density where $f(r) = 1$,

$$\overline{\psi^\dagger(r) \varphi(r)} + \overline{\varphi^\dagger(r) \psi(r)}. \quad (6.7)$$

this form of interference is very familiar in optics, equation (6.6) being the general case.

In particular, an abnormal form of single-particle interference can appear in the electron-pair amplitude,

$$\langle \psi_1(r) \psi_1(r) \rangle = \overline{[\psi_1(r) + \varphi_1(r)] [\psi_1(r) + \varphi_1(r)]}. \quad (6.8)$$
it is described by the abnormal cross terms
\[
\overline{\psi}_\uparrow(\mathbf{r})\varphi_\uparrow(\mathbf{r}) + \overline{\varphi}_\uparrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) + \overline{\psi}_\uparrow(\mathbf{r})\varphi_\uparrow(\mathbf{r}),
\] (6.9)
which have no counterparts in optics, in contrast to equation (6.7). From equation (3.3), one recognizes that the field \( \varphi(\mathbf{r}) \) contains two parts,
\[
\varphi(\mathbf{r}) = \varphi^{(+)}(\mathbf{r}) + \varphi^{(-)}(\mathbf{r}),
\] (6.10)
where \( \varphi^{(+)}(\mathbf{r}) \) represents the creation part,
\[
\varphi^{(+)}(\mathbf{r}) = \begin{bmatrix} \phi_\uparrow(\mathbf{r}) \\ \phi_\downarrow(\mathbf{r}) \end{bmatrix},
\] (6.11)
with \( \phi_\uparrow(\mathbf{r}) \) and \( \phi_\downarrow(\mathbf{r}) \) being connected with the operators \( c^\dagger_{k\uparrow} \) and \( c^\dagger_{k\downarrow} \), respectively; and \( \varphi^{(-)}(\mathbf{r}) \) the annihilation part, which is connected with the operators \( c_{-k\uparrow} \) and \( c_{-k\downarrow} \). This separation of two parts leads to
\[
\psi_\uparrow(\mathbf{r})\varphi_\uparrow(\mathbf{r}) + \overline{\varphi}_\uparrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) + \overline{\psi}_\uparrow(\mathbf{r})\varphi_\uparrow(\mathbf{r}) = \psi_\uparrow(\mathbf{r})\phi_\uparrow(\mathbf{r}) + \phi_\uparrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) + \varphi^{(-)}(\mathbf{r})\phi^\dagger_\uparrow(\mathbf{r}) + \phi^\dagger_\uparrow(\mathbf{r})\varphi^{(-)}(\mathbf{r}).
\] (6.12)
Clearly, there exists interference on the right-hand side; this interference induces the abnormal interference on the left-hand side. The abnormal interference has an important consequence; that is, the electrons are formed into Cooper pairs in the superconducting phase. Evidently, the abnormal interference vanishes in the normal phase.

Also, there exists two-particle interference in the superconducting phase, which arises from the statistical average of a two-body operator,
\[
\frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \langle \psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')v(\mathbf{r} - \mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}) \rangle = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' v(\mathbf{r} - \mathbf{r}')\overline{\psi}^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')\overline{\psi}(\mathbf{r}')\overline{\psi}(\mathbf{r}),
\] (6.13)
where \( v(\mathbf{r} - \mathbf{r}') \) stands for the two-body operator in the Schrödinger picture.

In the sense of equations (6.5) and (6.13), the superconducting phase can be identified as a form of interference pattern. Physically, the onset of an interference pattern will make a system more structured, and thus it increases its degree of order and decreases its entropy. That is why the superconducting phase has a higher degree of order and a lesser amount of entropy than the normal phase.

From the above discussions, it follows that there will appear interference in the ordered phase whereas there will not in the normal (disordered) phase. Obviously, the same conclusion holds for other phase transitions. Therefore, a phase transition amounts to the onset of a form of interference. As is well known, interference is a characteristic property of waves, and we thus conclude that phase transitions originate physically from the wave nature of matter.

Physically, any system will go in its disordered phase at sufficiently high temperatures, or as \( T \to +\infty \). Because the order parameter equals zero in the disordered phase, the extended ensemble theory should ensure that there exists a zero solution of the order parameter, at least at high temperatures. So it does, indeed.

doi:10.1088/1742-5468/2006/09/P09007
Upon a transformation, equation (2.6) can be expressed as
\[
S(\phi, \beta) = -\text{Tr} \left( \ln \left( \rho(H(c)) \right) \rho(H(c)) \right).
\]

Considering the expansion,
\[
e^{-iD(\phi, c)} H(c) e^{iD(\phi, c)} = H(c) - i[D(\phi, c), H(c)] + \frac{(-i)^2}{2} [D(\phi, c), [D(\phi, c), H(c)]] + \cdots,
\]
we obtain
\[
S(\phi, \beta) = -\text{Tr} \left( \ln \left( \rho(H(c)) \right) \rho(H(c)) \right)
+ \beta \frac{(-i)^2}{2} \text{Tr} \left( [D(\phi, c), [D(\phi, c), H(c)]] \rho(H(c)) \right) + \cdots,
\]
and the linear term of \( \phi \) vanishes.

Apart from an irrelevant term, this equation shows that the powers of \( \phi \) are equal to or higher than two in the expansion of \( S(\phi, \beta) \). As a result of \( \delta S = 0 \), the powers of \( \phi \) are equal to or higher than one in the equation of order parameter. This implies that there always exists a zero solution of \( \phi \) at any temperature, i.e., the trivial solution. In fact, this solution is a stable solution as \( T \to +\infty \),
\[
\Delta S = S(\delta \phi, \beta) - S(0, \beta) = -\text{Tr} \left( \ln \left( \rho(H(c)) \right) \left[ \rho(H'(\delta \phi, c)) - \rho(H(c)) \right] \right) = 0,
\]
\( T \to +\infty \)
which satisfies the criterion of equation (2.5). Of course, this conclusion is also valid for other phase transitions.

To summarize, there exists a zero solution of order parameter at any temperature in the extended ensemble theory; this solution becomes stable as \( T \to +\infty \). Therefore, a system always stays in its normal phase at sufficiently high temperatures; this high-temperature phase is disordered and structureless. As the temperature decreases, there can arise spontaneously the quantum interference of matter waves, which makes the system to become structured and transform into its ordered phase. That is the physical picture for phase transitions within the framework of the extended ensemble theory.

Remark. In [50], Yang suggested an important concept, i.e., off-diagonal long-range order (ODLRO), to describe quantum phase transitions. Physically, ODLRO is a generalization of the concept of Copper pairing. With this generalized concept, he developed many beautiful theorems, which are characteristics of quantum phases. Regrettably, in that paper, there is no discussion of the properties of the Hamiltonian that is needed to ensure the existence of ODLRO at low temperatures. Evidently, there exists no ODLRO if a system Hamiltonian is in its symmetric representation. The requirement can be satisfied if the system Hamiltonian takes its asymmetric, or broken-symmetry, representation. Therefore, those theorems in [50] still hold in the extended ensemble theory. As a matter of fact, the ODLROs of the reduced density matrices \( \rho_1 \) and \( \rho_2 \) [50], e.g., \( \text{Tr}(c_{\sigma\alpha} \rho(H'(\phi, c)) c_{\sigma}^\dagger) \) and \( \text{Tr}(c_{\alpha\sigma} c_{\sigma\alpha} \rho(H'(\phi, c)) c_{\sigma}^\dagger c_{\sigma}^\dagger) \), result physically from the single-particle and two-particle interferences, respectively. That is to say, off-diagonal long-range order is a physical manifestation of the quantum interference of matter waves.
7. Interacting Bose systems

In this section, we focus our attention on interacting Bose systems. We shall first study the weakly interacting Bose gas, and then the double-well potential systems where structural phase transitions, Goldstone bosons, and the Higgs mechanism are involved.

7.1. Weakly interacting Bose gas

As usual, the Hamiltonian for an interacting Bose gas reads

\[
H[\psi] = \int dr \left[ \frac{\hbar^2}{2m} \nabla \psi^\dagger(r) \cdot \nabla \psi(r) - \mu \psi^\dagger(r) \psi(r) \right] \\
+ \frac{1}{2} \int dr dr' \psi^\dagger(r) \psi^\dagger(r') v(r - r') \psi(r') \psi(r),
\]

where \( \psi(r) \) represents the boson-field operator, and \( v(r - r') \) the interaction. Expressed in terms of \( \psi(r) \) and \( \psi^\dagger(r) \), the phase-transition operator for BEC becomes

\[
D[\eta, \psi] = \int dr \left[ \eta^\dagger(r) \psi(r) + \eta(r) \psi^\dagger(r) \right].
\]

With \( H[\psi] \) and \( D[\eta, \psi] \), the entropy of the system can be obtained:

\[
S[\eta, \beta] = -\text{Tr} \left( \ln \left( \rho(H[\psi]) \right) \right) + \beta \left\{ \int dr \left[ \frac{\hbar^2}{2m} \nabla \eta^\dagger(r) \cdot \nabla \eta(r) - \mu \eta^\dagger(r) \eta(r) \right] \\
+ \int dr dr' \eta^\dagger(r) \eta(r') v(r - r') \overline{\psi^\dagger(r') \psi(r')} \\
+ \int dr dr' \eta^\dagger(r) \eta(r') v(r - r') \overline{\psi^\dagger(r') \psi(r)} \\
+ \frac{1}{2} \int dr dr' \eta^\dagger(r) \eta(r') v(r - r') \eta^\dagger(r') \eta(r') \right\},
\]

where \( \overline{F} \) denotes the statistical average of the operator \( F \) with respect to \( H[\psi] \). Its variation yields the equation of the order parameter,

\[
\left( -\frac{\hbar^2}{2m} \nabla^2 - \mu \right) \eta(r) + \int dr' \eta(r) v(r - r') \overline{\psi^\dagger(r') \psi(r')} + \int dr' \eta(r') v(r - r') \overline{\psi^\dagger(r) \psi(r)} \\
+ \int dr' \eta(r') v(r - r') \eta^\dagger(r') \eta(r') = 0.
\]

That is a generalized Ginzburg–Landau or Gross–Pitaevskii equation. In the simple case where \( v(r - r') = g \delta(r - r') \), it reduces to

\[
-\frac{\hbar^2}{2m} \nabla^2 \eta(r) + \left[ 2g \overline{\psi(r) \psi(r)} - \mu \right] \eta(r) + g |\eta(r)|^2 \eta(r) = 0,
\]

which is the standard Ginzburg–Landau [51] or Gross–Pitaevskii [52, 53] equation. In addition to equation (7.4), one also needs

\[
\int dr \eta^\dagger(r) \eta(r) + \int dr \overline{\psi^\dagger(r) \psi(r)} = N,
\]

doi:10.1088/1742-5468/2006/09/P09007
which is the equation of chemical potential. Equations (7.4) and (7.6) constitute the two basic equations for an interacting Bose system.

For simplicity, let us first consider the homogeneous solution,

$$\eta(r) = \xi,$$  \hspace{1cm} (7.7)

where \(\xi\) is independent of \(r\). Accordingly, equations (7.3) and (7.4) get simplified as

$$S[\eta, \beta] = -\text{Tr} \left( \ln \left( \rho(H[\psi]) \right) \right) + \beta \int \text{d}r \left[ -\tilde{\mu}\xi^\dagger \xi + \frac{1}{2}v(0)(\xi^\dagger \xi)^2 \right],$$  \hspace{1cm} (7.8)

$$-\tilde{\mu}\xi + v(0)|\xi|^2 \xi = 0,$$  \hspace{1cm} (7.9)

where

$$\tilde{\mu} = \mu - \int \frac{dk}{(2\pi)^3} \left[ v(0) + v(-k) \right] \left( \frac{1}{\beta\hbar} \right) \sum_n e^{i\omega_n \eta G(k, i\omega_n)},$$  \hspace{1cm} (7.10)

$$v(k) = \int \text{d}r v(r)e^{-ikr},$$  \hspace{1cm} (7.11)

\(G(k, i\omega_n)\) being the single-particle Green’s function defined with respect to \(H[\psi]\).

Equation (7.8) has the typical form of Landau free energy \[21\]. From equations (7.8), (7.9) and (2.5), it follows that the interaction between two particles must be repulsive for an interacting Bose system to be stable, i.e., \(v(r - r') > 0\). Otherwise, \(v(0) < 0\); the system will collapse.

Suppose that the repulsive interaction is weak; we can then treat it as a perturbation. As a technique of perturbation, we shall employ the GF tool, and adopt the self-consistent Hartree–Fock approximation as in \[54\],

$$\tilde{\varepsilon}(k) = \varepsilon(k) + \int \frac{dk'}{(2\pi)^3} \left[ v(k - k') - v(-k') \right] \left( \frac{1}{\beta\hbar} \right) \sum_n e^{i\omega_n \eta G(k', i\omega_n)},$$  \hspace{1cm} (7.13)

where \(\tilde{\varepsilon}(k)\) represents the proper self-energy. By use of equation (7.10), \(\mathcal{G}(k, i\omega_n)\) can be expressed as

$$\mathcal{G}(k, i\omega_n) = \frac{1}{i\omega_n - \hbar^{-1} \left[ \tilde{\varepsilon}(k) - \tilde{\mu} \right]},$$  \hspace{1cm} (7.14)

where

$$\mathcal{G}(k, i\omega_n) = \frac{1}{i\omega_n - \hbar^{-1} \left[ \tilde{\varepsilon}(k) - \tilde{\mu} \right]},$$  \hspace{1cm} (7.14)

$$\tilde{\varepsilon}(k) = \varepsilon(k) + \int \frac{dk'}{(2\pi)^3} \left[ v(k - k') - v(-k') \right] \left( \frac{1}{\beta\hbar} \right) \sum_n e^{i\omega_n \eta G(k', i\omega_n)}.$$  \hspace{1cm} (7.15)

Equation (7.14) shows that \(\tilde{\varepsilon}(k)\) and \(\tilde{\mu}\) are the renormalized energy and chemical potential, respectively.

With the help of equations (7.7) and (7.14), equation (7.6) can be reduced as

$$\xi^\dagger \xi + \int \frac{dk}{(2\pi)^3} \left( \frac{1}{\beta\hbar} \right) \sum_n e^{i\omega_n \eta G(k, i\omega_n)} = n,$$  \hspace{1cm} (7.16)

where \(n = N/V\) is the particle density of the system.
When $\tilde{\mu} < 0$, equation (7.9) has the only solution $\xi = 0$. As shown by equation (7.8), it is a stable solution. In this case, the system is in its normal phase. The renormalized chemical potential $\tilde{\mu}$ is given by equation (7.16),

$$
\mathcal{P} \int_{-\infty}^{+\infty} d\omega \, N(\omega, \tilde{\mu}) \frac{1}{e^{\beta \omega} - 1} = n,
$$

(7.17)

where $\mathcal{P}$ denotes the principal value introduced in appendix A, and $N(\omega, \tilde{\mu})$ the density of states,

$$
N(\omega, \tilde{\mu}) = -\int \frac{d\mathbf{k}}{(2\pi)^3} \text{Im} G(\mathbf{k}, \omega + i0^+).
$$

(7.18)

If $\tilde{\mu} > 0$, equations (7.8) and (7.9) show that the system will transform into a condensation phase where

$$
|\xi|^2 = \frac{\tilde{\mu}}{v(0)}.
$$

(7.19)

Substitution of it into equation (7.16) yields

$$
\frac{\tilde{\mu}}{v(0)} + \mathcal{P} \int_{-\infty}^{+\infty} d\omega \, N(\omega, \tilde{\mu}) \frac{1}{e^{\beta \omega} - 1} = n,
$$

(7.20)

which gives the renormalized chemical potential $\tilde{\mu}$ at $T < T_c$, where $T_c$ is the critical temperature for BEC,

$$
\mathcal{P} \int_{-\infty}^{+\infty} d\omega \, N(\omega, 0) \frac{1}{e^{\beta \omega} - 1} = n;
$$

(7.21)

that is to say, $\tilde{\mu}(T_c) = 0$. In sum, equations (7.17) and (7.20) yield together the renormalized chemical potential of the system at $T > T_c$ and $T < T_c$, respectively.

In order to deduce $\tilde{\mu}$ and $\xi$ in more detail, let us suppose further that $v(r - r')$ is of short range. Following [54], we can approximate $v(k)$ as

$$
v(k) = v(0) \left[ 1 - \frac{1}{6} (ka)^2 \right],
$$

(7.22)

where

$$
a^2 = \frac{\int d\mathbf{r} v^2(\mathbf{r})}{\int d\mathbf{r} v(\mathbf{r})}.
$$

(7.23)

Inserting equation (7.22) into equations (7.15) and (7.10) leads us to

$$
\tilde{\varepsilon}(k) = \frac{\hbar^2 k^2}{2m^*},
$$

(7.24)

$$
\tilde{\mu} = \mu - \left[ 2v(0) - \frac{v(0) nma^2}{3\hbar^2} m^* \right] \mathcal{P} \int_{-\infty}^{+\infty} d\omega \, N(\omega, \tilde{\mu}) \frac{(\omega + \tilde{\mu})}{e^{\beta \omega} - 1},
$$

(7.25)

where $m^*$ is the renormalized mass,

$$
\frac{1}{m^*} = \frac{1}{m} \left[ 1 - \frac{v(0) nma^2}{3\hbar^2} \left( 1 - \frac{|\xi|^2}{n} \right) \right],
$$

(7.26)
and $\mathcal{N}(\omega, \tilde{\mu})$ the density of states defined by equation (7.18),

$$
\mathcal{N}(\omega, \tilde{\mu}) = \begin{cases} 
\frac{1}{4\pi^2\hbar^3}(2m^*)^{3/2} (\omega + \tilde{\mu})^{1/2}, & \omega \geq -\tilde{\mu}, \\
0, & \omega < -\tilde{\mu}.
\end{cases}
$$

(7.27)

From equations (7.21), (7.26) and (7.27), it follows that

$$
\frac{T_c}{T_0} = 1 - \frac{v(0)nma^2}{3\hbar^2},
$$

(7.28)

where $T_0$ stands for the critical temperature of the BEC happening in the corresponding ideal Bose gas,

$$
T_0 = \frac{2\pi \hbar^2}{mk_B} \left( \frac{n}{\zeta (3/2)} \right)^{2/3}.
$$

(7.29)

Equation (7.28) manifests that a repulsive interaction will lower the transition temperature of BEC,

$$
\gamma \equiv \frac{\Delta T}{T_0} = \frac{T_c - T_0}{T_0} = -\frac{v(0)nma^2}{3\hbar^2} < 0.
$$

(7.30)

Also, we have by equation (7.17),

$$
\frac{2}{\sqrt{\pi}\zeta (3/2)} \int_0^{+\infty} dx \frac{x^{1/2}}{e^{x/\pi^2} - 1} = 1,
$$

(7.31)

where $t = T/T_c$ and $\overline{\mu} = \tilde{\mu}/(k_B T_c)$. This equation gives $\tilde{\mu}$ at $T > T_c$. If $T < T_c$, equation (7.20) must be used in place of equation (7.17),

$$
1 = y + \frac{2}{\sqrt{\pi}\zeta (3/2)} \left( \frac{1 + \gamma}{1 + \gamma - \gamma y} \right)^{3/2} \mathcal{P} \int_0^{+\infty} dx \frac{x^{1/2}}{e^{(x-y)/t} - 1},
$$

(7.32)

where $y = \tilde{\mu}/(v(0)n)$, and $\nu = v(0)n/(k_B T_c)$. This equation will yield both $\tilde{\mu}$ and $|\xi|^2 = \tilde{\mu}/v(0)$ at $T < T_c$.

The numerical results of $\tilde{\mu}$ and $|\xi|^2$ are shown in figures 4 and 5, respectively. We observe that the renormalized chemical potential $\tilde{\mu}$ is a monotonically decreasing function of temperature, at $T = T_c$ itself continuous but its derivative not. This agrees with the $T \geq T_c$ result given by [54] and the references therein. When $T < T_c$, the chemical potential $\tilde{\mu}$ is set zero in [54], as Einstein [45,46] did in the ideal Bose gas case. In the extended ensemble theory, there is no mathematical limit on $\tilde{\mu}$; it will change with temperature even if $T < T_c$ so as to ensure the conservation of particles, as pointed out in appendix A. The behaviour of $|\xi|^2$ shown in figure 5 is just expected for an order parameter.

The internal energy of the system, $E$, can be derived conveniently from $E = \langle H \rangle + \mu N$,

$$
\varepsilon = \nu + \frac{2}{\sqrt{\pi}\zeta (3/2)} \int_0^{+\infty} dx \frac{x^{3/2}}{e^{(x-\overline{\mu})/t} - 1}, \quad T \geq T_c,
$$

(7.33)

$$
\varepsilon = \nu - \frac{\overline{\mu}^2}{2\nu} + \frac{2}{\sqrt{\pi}\zeta (3/2)} \left( \frac{1 + \gamma}{1 + \gamma - \gamma y} \right)^{5/2} \mathcal{P} \int_0^{+\infty} dx \frac{x^{3/2}}{e^{(x-\overline{\mu})/t} - 1}, \quad T \leq T_c,
$$

(7.34)

doi:10.1088/1742-5468/2006/09/P09007
Figure 4. The chemical potential of the system versus temperature, where \( \mu = \tilde{\mu}/(k_B T_c) \), \( t = T/T_c \), \( \nu = v(0)n/\sqrt{\gamma T_c} \), and \( \gamma = \Delta T/T_0 = -v(0)nma^2/(3\hbar^2) \). For the sake of contrast, the chemical potential of the ideal Bose gas (\( \nu = 0, \gamma = 0 \)) is also plotted.

where
\[
\varepsilon = \frac{1}{k_B T_c} \frac{E}{N}.
\] (7.35)

Combination of equations (7.31) and (7.33) gives \( C_V \), the specific heat at constant volume,
\[
\frac{C_V}{Nk_B} = \frac{15}{4} \frac{g_{5/2}(z)}{g_{3/2}(z)} - \frac{9}{4} \frac{g_{3/2}(z)}{g_{1/2}(z)}, \quad T \geq T_c,
\] (7.36)
where
\[
z = e^{\tilde{\mu}/t},
\] (7.37)
\[
g_n(z) = \frac{1}{\Gamma(n)} \int_0^{+\infty} dx \frac{x^{n-1}}{z^{-1}e^x - 1}.
\] (7.38)

This result is the same in form as that for the ideal Bose gas, which is familiar in standard books on quantum statistical mechanics. If \( T \leq T_c \), \( C_V \) must be calculated from equations (7.32) and (7.34).

The numerical results of \( C_V \) are shown in figure 6. The shape of \( C_V \) shows that the BEC occurring in the interacting Bose gas is a ‘\( \lambda \)-transition’, as is naturally expected. In contrast to the ideal Bose gas, the weakly interacting Bose gas manifests itself with two new features: first, \( C_V \) is discontinuous at \( T = T_c \); and second, \( C_V \) is linear in temperature when \( T \ll T_c \). Evidently, this theoretical result for \( C_V \) meets the requirement of the third law of thermodynamics: \( C_V \to 0 \) as \( T \to 0 \). The discontinuity at \( T = T_c \) is obviously due
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Figure 5. The order parameter for BEC versus temperature, where $t = T/T_c$, $\nu = v(0)n/(k_B T_c)$, and $\gamma = \Delta T/T_0 = -v(0)ma^2/(3\hbar^2)$. For the sake of contrast, the order parameter for the ideal Bose gas ($\nu = 0$, $\gamma = 0$) is also plotted.

to the discontinuity of the derivatives of $\tilde{\mu}$ and $|\xi|^2$ with respect to $T$. As to the linearity at low temperatures, it can be explained as follows.

Observing that

$$
\mathcal{P} \int_0^{+\infty} dx \frac{x^{1/2}}{e^{(x-\nu y)/t} - 1} = - \int_0^{\nu y} x^{1/2} dx + t \int_0^{+\infty} dx \frac{(2\nu y + tx)^{1/2}}{e^{x+\nu y/t} - 1} + t \int_0^{\nu y/t} dx \frac{(\nu y + tx)^{1/2} - (\nu y - tx)^{1/2}}{e^x - 1},
$$

we obtain

$$
\mathcal{P} \int_0^{+\infty} dx \frac{x^{1/2}}{e^{(x-\nu y)/t} - 1} = -\frac{2}{3} (\nu y)^{3/2} + \zeta(2) (\nu y)^{-1/2} t^2,
$$

to the second power of $t$ as $t \ll 1$. Inserting it into equation (7.32), we have

$$
y = 1 - \frac{2}{\sqrt{\pi}\zeta(3/2)} \left( \frac{1 + \gamma}{1 + \gamma - \gamma y} \right)^{3/2} \left[ -\frac{2}{3} (\nu y)^{3/2} + \zeta(2) (\nu y)^{-1/2} t^2 \right],
$$

which is an iterative equation of $y$. At absolute zero ($t = 0$), it reduces to

$$
y_0 = 1 + \frac{4}{3\sqrt{\pi}\zeta(3/2)} \left( \frac{1 + \gamma}{1 + \gamma - \gamma y_0} \right)^{3/2} (\nu y_0)^{3/2}.
$$

This gives the zeroth order solution of $y$, which we denote by $y_0$. Iteration of equation (7.41) to the second power of $t$ leads to

$$
y = y_0 - \frac{2\zeta(2)}{\sqrt{\pi}\zeta(3/2)} \left( \frac{1 + \gamma}{1 + \gamma - \gamma y_0} \right)^{3/2} (\nu y_0)^{-1/2} t^2,
$$

doi:10.1088/1742-5468/2006/09/P09007
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Figure 6. The specific heat of a weakly interacting Bose gas versus temperature, where \( t = T/T_c \), \( \nu = v(0)n/(k_B T_c) \), and \( \gamma = \Delta T/T_0 = -v(0)nma^2/(3\hbar^2) \). For the sake of contrast, the specific heat of the ideal Bose gas \((\nu = 0, \gamma = 0)\) is also plotted.

which shows that \( y \), i.e., \( \tilde{\mu} \) and \( |\xi|^2 \), decreases as \( T^2 \) in the low-temperature region \((T \ll T_c)\), as can also be seen directly from figures 4 and 5. With the same procedure, one finds

\[
P \int_0^{+\infty} dx \frac{x^{3/2}}{e^{(x-\nu y)/t} - 1} = -\frac{2}{5} (\nu y)^{5/2} + 3\zeta(2)(\nu y)^{1/2} t^2. \tag{7.44}
\]

From equations (7.43), (7.44), and (7.34), it follows that \( \varepsilon \) increases as \( T^2 \). Therefore, the specific heat \( C_V \) will be linear in temperature \( T \) when \( T \ll T_c \).

If one expands equations (7.40) and (7.44) further to the fourth power of \( t \), one arrives at

\[
C_V = a(V)T + b(V)T^3, \tag{7.45}
\]

where the expansion coefficients \( a(V) \) and \( b(V) \) are functions of \( V \). Appendix B shows that this expansion does not depend on the approximations used here; it is valid provided that the interaction is weak. Therefore, it is a fundamental property of the weakly interacting Bose gas that the specific heat \( C_V \) vanishes linearly as \( T \to 0 \).

In connection with the \( \lambda \)-transition occurring in liquid \(^4\)He, obviously, the shape of \( C_V \) agrees well with that of the specific heat observed experimentally [55]. However, the latter is \( C_P \), the specific heat at constant pressure rather than at constant volume. As is well known from thermodynamics, they differ from each other by a temperature-dependent term,

\[
C_P = C_V + T \left( \frac{\partial p}{\partial T} \right)_V \left( \frac{\partial V}{\partial T} \right)_p. \tag{7.46}
\]
For solids at low temperatures,
\[ C_P \approx C_V, \]  
(7.47)
because
\[ \left( \frac{\partial V}{\partial T} \right)_P \approx 0. \]  
(7.48)
That is why the Debye \( T^3 \) law for the phonons, the \( T \) law for the electron gases in normal metals, and the exponential law for BCS superconductors are observed experimentally in \( C_P \) albeit they are the laws of \( C_V \) at low temperatures. In other words, the theoretical result of \( C_V \) for a solid can be verified straightforwardly by experiments. However, for a liquid, the situation is different: both the volume and pressure are much more sensitive to temperature. Therefore, the second term on the right-hand side of equation (7.46) cannot be neglected any longer; the difference between \( C_P \) and \( C_V \) becomes important and should be taken into account. As a result, to compare the theory with the experiment for a liquid, the experimental data for \( C_V \) or the theoretical result for \( C_P \) are needed. Regrettably, \( C_V \) is difficult to measure experimentally, and \( C_P \) is difficult to calculate theoretically. It is thus hard to compare the theoretical result with the experimental data. Fortunately, \( C_V \) tends to zero linearly as \( T \to 0 \) for a weakly interacting Bose gas, so we can compare the theoretical result with the experimental data in the limit \( T \to 0 \). That can be seen clearly from the following analyses.

According to the third law of thermodynamics, we have
\[ S_{th} = S_{th}(T, V) = \int_0^T C_V(T', V) \frac{dT'}{T'}, \]  
(7.49)
where, as pointed in section 2, \( S_{th} \) represents the thermodynamical entropy. Substituting equation (7.45) into this equation, we obtain
\[ S_{th} = a(V)T + \frac{1}{3}b(V)T^3, \]  
(7.50)
at low temperatures. Making use of the Maxwell relations,
\[ \left( \frac{\partial P}{\partial T} \right)_V = \left( \frac{\partial S_{th}}{\partial V} \right)_T, \]  
(7.51)
\[ \left( \frac{\partial V}{\partial T} \right)_P = - \left( \frac{\partial S_{th}}{\partial P} \right)_T, \]  
(7.52)
one has
\[ \left( \frac{\partial P}{\partial T} \right)_V = a'(V)T + \frac{1}{3}b'(V)T^3, \]  
(7.53)
\[ \left( \frac{\partial V}{\partial T} \right)_P = \left[ a'(V)T + \frac{1}{3}b'(V)T^3 \right]. \]  
(7.54)
Substituting them into equation (7.46) leads us to
\[ C_P = a(V)T + \tilde{b}(V)T^3, \]  
(7.55)
where the terms with power higher than cubic are omitted, and
\[ \tilde{b}(V) = b(V) - \left[ a'(V) \right]^2 \left( \frac{\partial V}{\partial P} \right)_T. \]  
(7.56)
Equation (7.55) presents the form of $C_P$ at low temperatures within the present theory. It contains a linear and a cubic term of $T$: the former includes only the contribution from $C_V$, and the latter includes both the contributions from $C_V$ and the second term on the right-hand side of equation (7.46). Heeding that $S_{\text{th}} = 0$ at $T = 0$, we have [56]

$$u^2 = -\frac{V^2}{mN} \left( \frac{\partial P}{\partial V} \right)_{T=0},$$

where $u$ denotes the velocity of sound. This implies that at low temperatures the velocity of sound is approximately

$$u^2 \approx -\frac{V^2}{mN} \left( \frac{\partial P}{\partial V} \right)_T.$$  

That is to say, the factor $(\partial V/\partial P)_T$ on the right-hand side of equation (7.56) represents physically the effect of sound. Therefore, the cubic term of $C_P$ includes the contribution from the sound, which is in accordance with the viewpoint of Landau on quantum Bose liquid He II [57, 58]. This $T^3$ law has already been observed experimentally in liquid $^4$He at low temperatures [55], but it is not an intrinsic property of the BEC because sound exists in all fluids. The intrinsic property of the BEC is the linear term of $C_P$: it comes purely from $C_V$, and is characteristic of a weakly interacting Bose gas at $T \ll T_c$, as mentioned above. There is no such linear term in the Landau theory of a quantum Bose liquid [57, 58]. To our knowledge, this linear behaviour of $C_P$ has not yet been reported experimentally for liquid $^4$He; it is thus a prediction of the present theory. Equation (7.55) indicates that the temperature $T$ has to go much lower for $C_P$ to show linear behaviour than to show the $T^3$ law. We believe that it would be observed if the measuring temperature is lowered enough, and if liquid $^4$He could be regarded as a weakly interacting Bose gas and the $\lambda$-transition were a Bose–Einstein condensation.

Remark. In general, $|\xi|^2$ cannot be interpreted as the density of condensed particles. This can be seen from equation (7.32); it shows that $y > 1$ at $T = 0$ K, that is,

$$|\xi|^2 > n$$

at absolute zero. However, in the case of the ideal Bose gas, $|\xi|^2$ cannot be greater than the density of particles, i.e.,

$$|\xi|^2 \leq n$$

at any temperature. Physically, $\xi$ is the order parameter and internal spontaneous field of the system; there is no a priori reason why it must be interpreted using the particle density. In fact, any statistical average of observable, including the particle density, will depend explicitly on $\xi$ when $T < T_c$.

Now, let us discuss the correlation of the BEC to the superfluidity. As usual, we set

$$\eta(r) = \sqrt{\rho(r)} e^{i\varphi(r)},$$

where $\rho(r) = |\eta(r)|^2$ and $\varphi(r) = \text{arg}(\eta(r))$. With this, we have

$$\mathbf{j}(r) = -\frac{i\hbar}{2m} \langle (\nabla - \nabla') \psi^\dagger(r) \psi(r') \rangle |_{r'=r}$$

$$= \frac{\hbar}{m} \rho(r) \nabla \varphi(r);$$

$$\text{doi:10.1088/1742-5468/2006/09/P09007}$$
obviously, \( j(\mathbf{r}) \) is the supercurrent density. If \( \varphi(\mathbf{r}) \), the phase of the BEC order parameter, is independent of \( \mathbf{r} \), there is no supercurrent: \( j(\mathbf{r}) = 0 \); otherwise, \( j(\mathbf{r}) \neq 0 \). The supercurrent velocity \( \mathbf{v} \) is given by

\[
\mathbf{v}(\mathbf{r}) = \frac{\hbar}{m} \nabla \varphi(\mathbf{r}).
\]  

(7.63)

Since the order parameter \( \eta(\mathbf{r}) \) is a single-valued function of the position \( \mathbf{r} \), we have

\[
\oint \mathbf{v}(\mathbf{r}) \cdot d\mathbf{r} = \frac{i\hbar}{m} l, \quad l \in \mathbb{Z}.
\]  

(7.64)

That is to say, there can exist quantized vortices in the condensed phase if \( \varphi(\mathbf{r}) \) depends on \( \mathbf{r} \). We remark that there exists a critical velocity \( v_c \); the velocity of the supercurrent cannot be greater than it, i.e., \( v \leq v_c \). That is because the increase of the supercurrent velocity is unfavourable to the decrease of the entropy of the system; the larger \( v \) is, the greater the entropy will be, which can be easily seen from the first integral over \( \mathbf{r} \) on the right-hand side of equation (7.3) with, e.g., \( \eta(\mathbf{r}) = \sqrt{\rho} e^{ik \cdot \mathbf{r}} \), where \( \rho = \text{constant} \).

Finally, we shall prove that there cannot exist any supercurrent or quantized vortex in the ideal Bose gas.

For the ideal Bose gas, \( v(\mathbf{r} - \mathbf{r'}) = 0 \), equation (7.4) reduces to

\[
-\frac{\hbar^2}{2m} \nabla^2 \eta(\mathbf{r}) = \mu \eta(\mathbf{r});
\]  

(7.65)

obviously, it is the eigenvalue equation of the kinetic energy operator. This equation can be rewritten as

\[
\frac{1}{2m} \int d\mathbf{r} [\mathbf{-i}\hbar \nabla \eta(\mathbf{r})] \cdot [\mathbf{-i}\hbar \nabla \eta(\mathbf{r})] = \mu \int d\mathbf{r} \eta(\mathbf{r}) \cdot \eta(\mathbf{r}).
\]  

(7.66)

This indicates that, for any nontrivial eigenfunction, the chemical potential \( \mu \) cannot be negative, i.e., \( \mu \geq 0 \). Therefore, there can only exist the trivial solution, \( \eta(\mathbf{r}) = 0 \), when \( \mu < 0 \). The nontrivial solution, \( \eta(\mathbf{r}) \neq 0 \), can exist only when \( \mu \geq 0 \) for the ideal Bose gas.

To discuss the stabilities of those solutions of equation (7.65), one needs to investigate whether \( \Delta S \geq 0 \). From equation (7.3), we find

\[
\Delta S = \beta \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} \nabla \delta \eta(\mathbf{r}) \cdot \nabla \delta \eta(\mathbf{r}) - \mu \delta \eta(\mathbf{r}) \delta \eta(\mathbf{r}) \right],
\]  

(7.67)

where \( \delta \eta(\mathbf{r}) \) represents the variation of the order parameter \( \eta(\mathbf{r}) \) from any one of the solutions of equation (7.65). Evidently, \( \Delta S \geq 0 \) when \( \mu \leq 0 \); this means that the system is stable when \( \mu \leq 0 \). Since \( \eta(\mathbf{r}) = 0 \) when \( \mu < 0 \) and \( \eta(\mathbf{r}) = \text{constant} \) when \( \mu = 0 \), the normal phase and the homogeneous condensed phase are both stable, which is in accordance with the results of section 5.1.2. As to the case of \( \mu > 0 \), the solution of equation (7.65) is inhomogeneous, which is just the case we are now interested in because an inhomogeneous solution can produce supercurrent and quantized vortices. To determine whether there can exist any supercurrent and quantized vortex in the condensed phase, we first reformulate the above equation as follows:

\[
\Delta S = \beta \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} \nabla^2 \right] \delta \eta(\mathbf{r}) - \mu \delta \eta(\mathbf{r}) \delta \eta(\mathbf{r})
\]  

(7.68)
and then examine the eigenvalue problem,

$$-\frac{\hbar^2}{2m} \nabla^2 \delta \eta(r) = E \delta \eta(r),$$

(7.69)

$$\delta \eta(r)|_{r \to \infty} = 0.$$ (7.70)

Equation (7.70) is the boundary condition obeyed by the variation $\delta \eta(r)$. Obviously, this eigenvalue problem always has solutions when $E > 0$, e.g.,

$$\delta \eta(r) = j_l(kr), \quad k = \sqrt{\frac{2m}{\hbar^2}} E,$$

(7.71)

where $j_l(z)$ is the spherical Bessel function. Accompanying those solutions, $\Delta S$ can be reexpressed as

$$\Delta S = \beta \int dr (E - \mu) \delta \eta^\dagger(r) \delta \eta(r);$$ (7.72)

clearly,

$$\Delta S > 0, \quad E > \mu,$$

$$\Delta S = 0, \quad E = \mu,$$

$$\Delta S < 0, \quad E < \mu.$$ (7.73)

This shows that any solution of equation (7.65) for $\mu > 0$ belongs to the saddle points of the system entropy. In other words, any inhomogeneous condensed phase is physically unstable: needless to say, the supercurrent and quantized vortex. This proves that there cannot exist any supercurrent or quantized vortex in the ideal Bose gas.

By the way, the above analyses demonstrate that the condensed phase of the ideal Bose gas must be homogeneous. There is no inhomogeneous condensation in the ideal Bose gas. This result is very natural, and it confirms Einstein’s deep physical insight on BEC, again.

### 7.2. Double-well potential and the BEC in configuration space

From section 5.3, it is learned that an ideal phonon gas cannot produce BEC. However, the ideal phonon gas is simply a harmonic approximation to an actual solid. Generally, the interatomic interaction is anharmonic. This thus raises the question as to whether or not an anharmonic system can produce BEC. We intend to discuss the question in this subsection.

To that end, it is helpful to make a representation transformation to the formulation used in section 5.3. There, what we used is the Fock space where all the observables are expressed in terms of creation and annihilation operators. In the following, we prefer to use the phase space where all the observables are expressed in terms of generalized coordinates and momenta. As is well known, the two spaces are equivalent and can be transformed into each other according to such a rule as [59]

$$q_i = \sqrt{\frac{\hbar}{2m_i \omega_i}} (a_i + a_i^\dagger),$$

$$p_i = -i \sqrt{\frac{m_i \hbar \omega_i}{2}} (a_i - a_i^\dagger),$$

(7.74)
and

\begin{align}
  a_i &= \sqrt{\frac{m_i \omega_i}{2\hbar}} q_i + \frac{i}{\sqrt{2m_i \hbar \omega_i}} p_i, \\
  a_i^\dagger &= \sqrt{\frac{m_i \omega_i}{2\hbar}} q_i - \frac{i}{\sqrt{2m_i \hbar \omega_i}} p_i,
\end{align}

(7.75)

where \(q_i\) and \(p_i\) are the \(i\)th pair of coordinate and momentum; \(a_i\) and \(a_i^\dagger\) the corresponding annihilation and creation operators; \(m_i\) the effective mass; and \(\omega_i > 0\) the \(i\)th parameter, which can generally take any positive value, and particularly the natural frequency if \(q_i\) and \(p_i\) constitute a harmonic oscillator. Along with equations (7.74) and (7.75), the main quantities concerned are transformed as follows:

\begin{align}
F(a) &\iff F(q,p), \\
H(a) &\iff H(q,p), \\
D(\xi,a) &\iff D(\eta,\zeta,q,p), \\
S(\xi,\beta) &\iff S(\eta,\zeta,\beta),
\end{align}

(7.76) (7.77) (7.78) (7.79)

where

\begin{align}
D(\xi,a) &= \sum_i (\xi_i^\dagger a_i + \xi_i a_i^\dagger), \\
D(\eta,\zeta,q,p) &= \frac{1}{\hbar} \sum_i (\eta_i q_i + \zeta_i p_i), \\
\eta_i &= \sqrt{\frac{m_i \hbar \omega_i}{2}} (\xi_i^\dagger + \xi_i), \\
\zeta_i &= i \sqrt{\frac{\hbar}{2m_i \omega_i}} (\xi_i^\dagger - \xi_i).
\end{align}

(7.80) (7.81) (7.82)

Here, \(\xi\) represents the order parameter for BEC in Fock space, \(\eta_i\) and \(\zeta_i\) the corresponding order parameters in phase space.

Under the action of \(D(\eta,\zeta,q,p)\), the statistical averages of \(q_i\) and \(p_i\) will change with temperature as

\begin{align}
\langle q_i \rangle &= -\zeta_i + \text{Tr} (q_i \rho (H(q,p))), \\
\langle p_i \rangle &= \eta_i + \text{Tr} (p_i \rho (H(q,p))).
\end{align}

(7.83)

If the system produces a BEC, i.e., \(\eta_i\) and/or \(\zeta_i\) change from zero to nonzero with the decreasing of temperature, the average positions of the particles will redistribute in phase space. In this sense, the BEC is said to be the phase-space BEC: it changes the distribution of the system in phase space. If, however, the BEC only causes \(\eta_i\) (or \(\zeta_i\)) to change from zero to nonzero, the particles will redistribute merely in momentum space (or configuration space), the subspace of phase space. In such a case, the BEC is said to be the momentum-space BEC (or the configuration-space BEC): it changes only the distribution of the system in momentum space (or configuration space). Obviously, once a BEC changes the distribution of a system in configuration space (\(\zeta_i \neq 0, \eta_i = 0\) or not), it induces a
structural phase transition (SPT) [60]. In this connection, it can be said that an SPT is just an instance of BEC.

Commonly, a system Hamiltonian has the form

\[ H(q, p) = \sum_i \frac{p_i^2}{2m_i} + \sum_i u(q_i) + \frac{1}{2} \sum_{i,j} v(q_i - q_j), \]  

(7.84)

where \( u(q_i) \) and \( v(q_i - q_j) \) stand for the single- and two-particle potentials, respectively. One can easily verify, using equations (2.4), (2.5), (7.78) and (7.79), that \( \eta_i \) must be zero at any temperature, i.e., there cannot arise the momentum-space BEC. In consequence, the system with such a form of Hamiltonian can, at most, produce a configuration-space BEC. Therefore, an SPT is commonly a configuration-space BEC. In the following, we shall confine our attention to this kind of SPT. The phase-transition operator \( D(\eta, \zeta, q, p) \) can now be simplified as

\[ D(\zeta, p) = \frac{1}{\hbar} \sum_i \zeta p_i, \]  

(7.85)

for \( \eta_i \) vanishes forever.

In the field of SPTs, the Hamiltonian of equation (7.84) is made concrete as [60]

\[ H(q, p) = \sum_i \frac{p_i^2}{2m_i} + \sum_i \left( \frac{1}{2} \mu^2 q_i^2 + \frac{1}{4} g q_i^4 \right) + \sum_{(ij)} \frac{1}{2} \lambda (q_i - q_j)^2, \]  

(7.86)

where \( \mu^2, g, \) and \( \lambda \) are constants, and \( \langle ij \rangle \) denotes the nearest neighbour sites. The system becomes anharmonic if \( \mu^2 < 0 \) or \( g \neq 0 \). The terms included by the second sum represent the single-particle potential that arises from an underlying sublattice of atoms, which do not participate actively in the phase transition, and the one included by the third sum represents the elastic coupling between nearest neighbours, which is described by a harmonic potential with the coupling constant \( \lambda \geq 0 \). Obviously, \( H(q, p) \) has the discrete symmetry

\[ q_i \rightarrow q_i' = \exp \left( \frac{i}{\hbar} \sum_i \left( \frac{1}{2} p_i^2 + \frac{1}{2} q_i^2 \right) \right) q_i \exp \left( -\frac{i}{\hbar} \sum_i \left( \frac{1}{2} p_i^2 + \frac{1}{2} q_i^2 \right) \right) = -q_i; \]  

(7.87)

this leads us to

\[ \overline{q_i} = 0, \]  

(7.88)

where

\[ \overline{F(q, p)} = \text{Tr} (F(q, p) \rho (H(q, p))). \]  

(7.89)

This discrete symmetry will break down if an SPT takes place.

Let us begin with the simple case of \( \lambda = 0 \). Making use of equation (7.85), we have

\[ S(\zeta, \beta) = -\ln (\rho (H(q, p))) + \beta \sum \left\{ \frac{1}{2} \left[ \mu^2 + 3g \left( \overline{q_i^2} - \overline{q_i}^2 \right) \right] \zeta_i^2 + \frac{1}{4} g \zeta_i^4 \right\}. \]  

(7.90)

This shows that the entropy \( S(\zeta, \beta) \) has the typical form of Landau free energy [21]. From equations (7.90), (2.4), and (2.5), one can draw three conclusions.
(1) The case of \( g < 0 \). The system is unstable and will collapse because the entropy is unbounded from below with respect to the variation of \( \zeta \).

(2) The case of \( g = 0 \).
   (a) If \( \mu^2 > 0 \), the trivial solution \( \zeta_i = 0 \) is the only minimizer of \( S(\zeta, \beta) \). That is to say, a system consisting of harmonic oscillators, or rather an ideal phonon gas, cannot produce an SPT; it will stay in the normal phase forever, which is in accordance with the result of section 5.3.
   (b) If \( \mu^2 = 0 \), \( \zeta_i \) can take a temperature-independent value; it represents, as indicated by equations (7.83) and (7.88), the equilibrium position of \( q_i \), i.e., \( \langle q_i \rangle = -\zeta_i \). As the initial equilibrium position of \( q_i \) at \( \beta = 0 \), \( -\zeta_i \) can be chosen as zero. Therefore, a system composed of free distinguishable particles cannot produce an SPT, as is just expected.
   (c) If \( \mu^2 < 0 \), \( \zeta_i = 0 \) is the only solution, but it is a maximizer of \( S(\zeta, \beta) \), the system is unstable and will collapse. This result is quite natural since all particles go in a reversed harmonic potential.

(3) The case of \( g > 0 \).
   (a) If \( \mu^2 \geq 0 \), \( \zeta_i = 0 \) is the only solution, and it is a minimizer of \( S(\zeta, \beta) \). There is no phase transition in the system; the potential is a single well.
   (b) If \( \mu^2 < 0 \), the potential becomes double-welled, and it must be determined by the position fluctuation \( q_i^2 - \bar{q}_i^2 \) whether or not the system can produce a phase transition. Evidently, a transition can occur if the fluctuation is such a decreasing function of temperature that \( \mu^2 + 3g(q_i^2 - \bar{q}_i^2) \) can change in sign, from positive to negative. If the fluctuation is so strong that \( \mu^2 + 3g[(q_i^2) - (\bar{q}_i)^2] > 0 \) up to zero temperature, the system has to stay in the normal phase forever.

From the above discussions, it follows that a double-well potential where \( \mu^2 < 0 \) and \( g > 0 \) is the only possible case for the system to produce a structural phase transition under the condition of \( \lambda = 0 \). One can easily verify that this conclusion is still valid for \( \lambda > 0 \).

We are now confronted with performing the evaluation of the position fluctuation \( q_i^2 - \bar{q}_i^2 \) so as to ascertain whether or not a phase transition can occur if \( \mu^2 < 0 \) and \( g > 0 \). To this end, we need to perform a representation transformation to the Hamiltonian of equation (7.86) because, as is well known, this form of Hamiltonian has no good basic part and is thus unfavourable for making approximations. Complying with quantum field theory, the transformation can be achieved as follows:

\[
q_i \mapsto \phi_i = \exp \left( \frac{i}{\hbar} \sum_j \nu p_j \right) q_i \exp \left( \frac{-i}{\hbar} \sum_j \nu p_j \right) = qi + \nu,
\]

\[
p_i \mapsto \pi_i = \exp \left( \frac{i}{\hbar} \sum_j \nu p_j \right) p_i \exp \left( \frac{-i}{\hbar} \sum_j \nu p_j \right) = pi,
\]

where

\[
\nu = \sqrt{-\mu^2/g}.
\]

In the sense of classical mechanics, the above transformation amounts to performing a translation so that the new coordinate \( \phi_i \) is referenced from \( q_i = -\nu \), one of the two minimizers of the double-well potential. Along with equation (7.91), the new
representation $H(\phi, \pi)$ of the Hamiltonian becomes

$$H(\phi, \pi) = \exp \left( \frac{\imath}{\hbar} \sum_j \nu p_j \right) H(q, p) \exp \left( -\frac{\imath}{\hbar} \sum_j \nu p_j \right)$$

$$= \sum_i \left( \frac{p_i^2}{2m} - \mu^2 q_i^2 \right) + \sum_i \left( g \nu q_i^3 + \frac{1}{4} g \nu^4 \right) - \sum_i \frac{1}{4} g \nu^4.$$

(7.93)

The first sum on the right-hand side represents harmonic oscillators with natural frequencies $\omega_i = \sqrt{-2\mu^2/m}$; it constitutes a basic Hamiltonian which is favourable for approximation handling; the second sum is the interaction, and the third is an unimportant constant.

With $H(\phi, \pi)$, one finds

$$\tilde{q}^2 - \tilde{q}^2 = \tilde{\phi}^2 - \tilde{\phi}^2 = \tilde{q}^2 - \tilde{q}^2,$$

(7.94)

where $\tilde{F}$ stands for the statistical average with respect to $H(\phi, \pi)$,

$$\tilde{F} = \text{Tr} \left( F(q, p) \rho(H(q, p)) \right),$$

(7.95)

where $\tilde{H}(q, p) = H(\phi, \pi)$. According to equation (7.94), we now just need to evaluate the fluctuation $\tilde{q}^2 - \tilde{q}^2$; it can be worked out by the retarded Green’s function $\langle \langle q_i | q_i \rangle \rangle_\omega$ which is defined with respect to $\tilde{H}(q, p)$ [39]. The Green’s function satisfies the following equation of motion:

$$\hbar \omega \langle \langle q_i | q_i \rangle \rangle_\omega = \langle \langle q_i, q_i \rangle \rangle + \langle \langle q_i, \tilde{H}(q, p) | q_i \rangle \rangle_\omega$$

$$= \frac{\imath \hbar}{m} \langle \langle p_i | q_i \rangle \rangle_\omega.$$ 

(7.96)

Also,

$$\hbar \omega \langle \langle p_i | q_i \rangle \rangle_\omega = \langle \langle p_i, q_i \rangle \rangle + \langle \langle p_i, \tilde{H}(q, p) | q_i \rangle \rangle_\omega$$

$$= -\imath \hbar [1 - 2\mu^2 \langle \langle q_i | q_i \rangle \rangle_\omega + 3g \nu \langle \langle q_i^3 | q_i \rangle \rangle_\omega + g \langle \langle q_i^3 | q_i \rangle \rangle_\omega].$$ 

(7.97)

We would like to truncate the GF chain with the following decoupling approximation:

$$\langle \langle q_i^2 | q_i \rangle \rangle_\omega = \tilde{q}_i \langle \langle q_i | q_i \rangle \rangle_\omega = -\nu \langle \langle q_i | q_i \rangle \rangle_\omega,$$

(7.98)

$$\langle \langle q_i^3 | q_i \rangle \rangle_\omega = \tilde{q}_i^2 \langle \langle q_i | q_i \rangle \rangle_\omega = \left[ (q_i^2 - \tilde{q}_i^2) + \nu^2 \right] \langle \langle q_i | q_i \rangle \rangle_\omega,$$

(7.99)

where we have used the result $\tilde{\phi}_i = \tilde{q}_i + \nu = 0$, which follows from equation (7.88). This approximation leads us to

$$\langle \langle q_i | q_i \rangle \rangle_\omega = \frac{1}{m \omega^2 - \omega_s^2},$$

(7.100)

where

$$\omega_s = \left[ \frac{3g}{m} (\tilde{q}_i^2 - \tilde{q}_i^2) \right]^{1/2}$$

(7.101)

represents the renormalized frequency. According to the fluctuation-dissipation theorem [39], the fluctuation $\tilde{q}_i^2 - \tilde{q}_i^2$ can be obtained by

$$\tilde{q}_i^2 - \tilde{q}_i^2 = \mathcal{P} \int_{-\infty}^{+\infty} d\omega \frac{1}{\text{e}^{\hbar \omega} - 1} \left[ -\frac{\hbar}{\pi} \text{Im} \langle \langle q_i | q_i \rangle \rangle_{\omega + \imath \nu} \right].$$

(7.102)
it gives rise to
\[ \overline{q_i^2} - q_i^2 = \frac{\hbar}{m\omega_s} \left( \frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_s} - 1} \right). \] (7.103)

Equations (7.103) and (7.101) constitute a self-consistent approximation to the fluctuation \( \overline{q_i^2} - q_i^2 \). Evidently, the first term on the right-hand side of equation (7.103) represents the zero-point fluctuation. Equation (7.103) shows that the fluctuation gets weaker when the temperature goes lower. At zero temperature, one has
\[ \overline{q_i^2} - q_i^2 = \frac{1}{\sqrt{4mg}} \hbar^{2/3} \sim O(\hbar^{2/3}), \] (7.104)
and at high temperatures,
\[ \overline{q_i^2} - q_i^2 = \frac{1}{\sqrt{g\beta}} \sim O(T^{1/2}). \] (7.105)

These imply that there exists a finite temperature \( T_c \) such that
\[
\begin{align*}
\mu^2 + 3g(\overline{q_i^2} - q_i^2) &> 0, & T > T_c, \\
\mu^2 + 3g(\overline{q_i^2} - q_i^2) &= 0, & T = T_c, \\
\mu^2 + 3g(\overline{q_i^2} - q_i^2) &< 0, & T < T_c.
\end{align*}
\] (7.106)

From equations (7.106) and (7.90), it follows that an SPT will occur at \( T_c \),
\[ \zeta_i = \begin{cases} 0, & T \geq T_c, \\ \pm \left[ -\frac{\mu^2}{g} - \frac{3\hbar}{m\omega_s} \left( \frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_s} - 1} \right) \right]^{1/2}, & T < T_c. \end{cases} \] (7.107)

Specifically, \( \zeta_i = \pm \sqrt{-\mu^2/g} \) at zero temperature if the zero-point fluctuation is neglected, i.e., the order parameter will equal one of the two minimizers of the double-well potential at zero temperature when the zero-point fluctuation is left out of consideration.

Combining equations (7.107), (7.83), and (7.88), we have
\[ \langle q_i \rangle = \begin{cases} 0, & T \geq T_c, \\ \pm \left[ -\frac{\mu^2}{g} - \frac{3\hbar}{m\omega_s} \left( \frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_s} - 1} \right) \right]^{1/2}, & T < T_c. \end{cases} \] (7.108)

This shows that for each site the distortion \( \langle q_i \rangle \) can take independently either of the two values at \( T < T_c \). There is no correlation between the distortions of different sites; therefore, the new phase below \( T_c \) is a structural glass. Physically, that is because we have discarded the coupling between nearest neighbours (\( \lambda = 0 \)). If it is taken into account (\( \lambda > 0 \)), one can easily verify that the new phase below the transition temperature will be ferrodistortive:
\[ \langle q_i \rangle = \langle q_j \rangle, \] (7.109)
where \( i \) and \( j \) denote any two different sites. This result is in agreement with the classical mean-field theory [60].

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In conclusion, we find that the double-well potential system described by the Hamiltonian of equation (7.86) can produce a structural phase transition. Mechanically, that is because the position fluctuations of particles will decrease with temperature. In the high-temperature regime, the fluctuations are relatively strong, and the system can only stay in its normal phase. The fluctuations will get weaker when temperature goes lower, and finally the system undergoes a transition at a finite temperature and then turns into a new ordered phase in the low-temperature regime. We learn from this that the position fluctuations of particles play an important role in structural phase transitions. Also, we see that configuration space is very convenient for describing an SPT, in contrast to the Fock space.

7.3. Goldstone bosons, Ginzburg–Landau equations, and Higgs mechanism

Obviously, the preceding theory for the discrete case can be extended straightforwardly to the continuum case. Let us consider the so-called O($\mathbf{N}$)-symmetric vector model [61,62],

$$H[\psi, \pi] = \int \! \! \! d\! x \left\{ \frac{1}{2} \pi^\dagger \pi + \frac{1}{2} \nabla \psi^\dagger \cdot \nabla \psi + \frac{m^2}{2} \psi^\dagger \psi + \frac{g}{4} (\psi^\dagger \psi)^2 \right\}, \quad (7.110)$$

where $m^2 < 0$ and $g > 0$ are the two constant parameters for a double-well potential, $\psi(x)$ is usually called the Higgs field (it represents a real-valued vector field with $N$ components), and $\pi(x)$ the corresponding momentum,

$$[\psi_i(x), \pi_j(x')] = i \delta_{ij} \delta(x - x'). \quad (7.111)$$

As is well known, this double-well Hamiltonian is the typical model for SSB in quantum field theory [61]–[63]. The arguments given in the preceding subsection are still valid. They reveal that the physical reason why the O($\mathbf{N}$) symmetry will break down is that the fluctuation of the field $\psi(x)$ decreases monotonically with temperature, and that this SSB belongs essentially to the BEC happening in configuration space.

In the condensation phase, the system Hamiltonian takes the form

$$H'[\varphi, \psi, \pi] = e^{iD[\varphi, \pi]} H[\psi, \pi] e^{-iD[\varphi, \pi]}, \quad (7.112)$$

where $\varphi(x)$ is the order parameter for the Higgs field, and $D[\varphi, \pi]$ the phase-transition operator,

$$D[\varphi, \pi] = \int \! \! \! d\! x \varphi^\dagger(x) \pi(x). \quad (7.113)$$

In more detail, equation (7.112) can be written as

$$H'[\varphi, \psi, \pi] = \int \! \! \! d\! x \left\{ \frac{1}{2} \pi^\dagger \pi + \frac{1}{2} \nabla (\psi^\dagger + \varphi^\dagger) \cdot \nabla (\psi + \varphi) + \frac{m^2}{2} (\psi^\dagger + \varphi^\dagger)(\psi + \varphi) 
+ \frac{g}{4} [(\psi^\dagger + \varphi^\dagger)(\psi + \varphi)]^2 \right\}. \quad (7.114)$$

At absolute zero, if one neglects the zero-point fluctuation of the field $\psi$, i.e., $\overline{\psi^\dagger \psi} \approx 0$, then one has the stable solution,

$$\varphi^\dagger \varphi = \nu^2, \quad (7.115)$$

doi:10.1088/1742-5468/2006/09/P09007
where
\[ \nu = \sqrt{-m^2/g} \]  
(7.116)
is the minimizer of the double-well potential. Without loss of generality, we shall take
\[ \phi^\dagger = [\nu, 0, \ldots, 0]. \]  
(7.117)
Substituting this into equation (7.114) leads us to
\[
H'[\phi, \psi, \pi] = \int dx \left[ \frac{1}{2} \pi^\dagger \pi + \frac{1}{2} \nabla \phi^\dagger \cdot \nabla \phi - m^2 \psi_1^2 + \frac{g}{4} (\psi^\dagger \psi)^2 - \frac{g\nu}{4} \right].
\]  
(7.118)
That is the zero-temperature representation of the system Hamiltonian; it shows that the first component field \( \psi_1(x) \) gets a mass of \(-2m^2\); the others are massless. As is well known, those massless particles are the so-called Goldstone bosons [64]. From here, one can see how Goldstone bosons are produced in a natural way by spontaneous symmetry breaking within the framework of the extended ensemble theory. Of course, one should also recognize that the zero-point fluctuation can impose a little influence on the Goldstone bosons.

Finally, it should be emphasized that, in the O(\(N\))-symmetric vector model, Goldstone bosons originate physically from the Bose–Einstein condensation of the Higgs field.

If a gauge field is coupled with the Higgs field \( \psi(x) \), what will happen to the gauge field? Can it produce BEC as the Higgs field \( \psi(x) \)? To clarify this problem, let us consider, for simplicity, the coupling of a complex-valued (or two-component) Higgs field \( \psi(x) \) and an electromagnetic field \( A(x) \),
\[
H[\psi, \pi; A, E] = \int dx \left[ \pi^\dagger \pi + (\nabla + ieA) \psi^\dagger \cdot (\nabla - ieA) \psi + m^2 \psi_1^2 + \frac{g}{4} (\psi^\dagger \psi)^2 \right.
\]
\[+ \frac{1}{2} E^2 + \frac{1}{2} (\nabla \times A)^2, \tag{7.119} \]
where \( e \) is the charge of the Higgs field \( \psi(x) \), and \( E(x) \) the electric field strength which plays the role of the canonical momentum corresponding to the canonical coordinate \( A(x) \),
\[
[A_i(x), -E_j(x')] = i\delta_{ij}\delta(x - x'). \tag{7.120} \]
Here, the temporal gauge has been used to perform a canonical quantization to the electromagnetic field, an Abelian gauge field. The reason for choosing this gauge is that it can be easily applied to quantize non-Abelian gauge fields, and transformed into other gauges through the path-integral formalism introduced by Faddeev and Popov [65].

For this coupled system, BEC can be explored through the phase-transition operator,
\[
D[\phi, \pi; A, E] = \int dx \left( \phi \pi^\dagger - \phi^\dagger \pi - A \cdot E \right), \tag{7.121} \]
where $\varphi(x)$ and $\Lambda(x)$ are the order parameters for the Higgs field $\psi(x)$ and gauge field $A(x)$, respectively. With $D[\varphi, \pi; \Lambda, E]$, one can obtain the entropy of the system,

$$S[\varphi, \Lambda, \beta] = - \text{Tr} \left( \ln(\rho(H[\psi, \pi; A, E]))\rho(H[\psi, \pi; A, E]) \right) + \int dx \left[ (\nabla + ie\Lambda)^\dagger (\nabla - ie\Lambda) \varphi + (m^2 + e^2 A \cdot A + 4g\psi^\dagger \psi) \varphi^\dagger \varphi + g (\varphi^\dagger \varphi)^2 + e^2 \psi^\dagger \psi \Lambda^2 + \frac{1}{2} (\nabla \Lambda)^2 \right],$$

(7.122)

which shows that the two order parameters $\varphi$ and $\Lambda$ are coupled together. Equation (7.122) reminds us of the Landau free energy for superconductivity [51, 56]; indeed, they are both similar in form.

Variation of $S$ with respect to $\varphi$ and $\Lambda$ yields

$$- (\nabla - ie\Lambda)^2 \varphi + (m^2 + e^2 A \cdot A + 4g\psi^\dagger \psi) \varphi + 2g\varphi^\dagger \varphi \varphi = 0,$$

(7.123)

$$\nabla \times \nabla \times \Lambda = -ie \left( (\varphi^\dagger \nabla \varphi - \varphi \nabla \varphi^\dagger) - 2e^2 (\varphi^\dagger \varphi + \psi^\dagger \psi) \Lambda \right).$$

(7.124)

This form of two coupled nonlinear equations is known as Ginzburg–Landau equations [51, 56]. Observing that

$$\langle B \rangle = -\nabla \times A,$$

(7.125)

where $B$ denotes the magnetic field strength, one can specify

$$\nabla \cdot A = 0,$$

(7.126)

which indicates that there are only two independent order parameters for the electromagnetic field. Equation (7.126) can be regarded as the Coulomb gauge to the vector order parameter $A$.

From equations (7.122)–(7.126), one can easily verify that there is no BEC for the electromagnetic field $A$ if it is not coupled with the Higgs field $\psi$, or it is coupled with $\psi$ but the latter has not condensed yet ($\varphi = 0$). This also confirms the conclusion of section 5.3: an ideal photon gas, or a free electromagnetic filed, cannot produce BEC. Once the Higgs field $\psi$ gets condensed ($\varphi \neq 0$), the electromagnetic field $A$ must condense down ($\Lambda \neq 0$) simultaneously; otherwise, there can arise a linear term of $\delta \Lambda$ in $\delta S$, and the coupled system will become unstable. This shows that the gauge field $A$ will condense together with the Higgs fields $\psi$ when it is coupled with the latter. In such a case, the transition is cooperative; one usually says that $\varphi$ is the primary order parameter, and $\Lambda$ the secondary one.

With the help of equations (7.126), (7.124) can be reduced as

$$\nabla^2 \Lambda - 2e^2 (\varphi^\dagger \varphi + \psi^\dagger \psi) \Lambda = -ie (\varphi^\dagger \nabla \varphi - \varphi \nabla \varphi^\dagger).$$

(7.127)

Heeding that $\langle A \rangle = -\Lambda$, equation (7.127) is identical to the static Proca equation [66] except that the prefactor of $\Lambda$ may be a function of $r$; the counterpart in the Proca equation just a constant. In general, the prefactor cannot be interpreted as the mass of the gauge field. However, once there is a constant occurring in the prefactor, a mass $\mu$ is generated to the gauge field, as can be seen more clearly in the following discussion.

Owing to the nonlinearity, the Ginzburg–Landau equations (7.123) and (7.124) are rather complicated to handle. As usual, let us consider the zeroth-order approximation of equation (7.123) at $T = 0$ K [51, 56],

$$\varphi^\dagger(x) \varphi(x) = \nu^2 / 2,$$

(7.128)

doi:10.1088/1742-5468/2006/09/P09007
where the effect of $\mathbf{A}$ and the zero-point fluctuations of the fields $\psi$ and $\mathbf{A}$ are omitted. From equations (7.127) and (7.128), it follows that
\[
\nabla^2 \langle \mathbf{A} \rangle - e^2 \nu^2 \langle \mathbf{A} \rangle = 0.
\]
(7.129)
Since the prefactor $e^2 \nu^2$ is constant now, it can be interpreted as the mass of the gauge field at zero temperature,
\[
\mu^2 (T = 0) = e^2 \nu^2.
\]
(7.130)
As is well known, this mass can account for the Meissner effect [67], i.e., the expulsion of a magnetic field from the interior of a superconducting material, with a London penetration length $\lambda_L = \mu^{-1} [68]$.

The above formalism is the Ginzburg–Landau picture of creation of mass; in this picture, the mass is represented by the equation of motion. There is another picture, which is due to Higgs [69]–[71]. In the Higgs picture, the mass is represented directly by the system Hamiltonian itself. Since an equation of motion is in accordance with its equation of motion, we consider the zero-temperature representation $H_0$ of the system Hamiltonian,
\[
H_0 = e^{iD[\varphi, \pi; \mathbf{A}, \mathbf{E}]} H [\psi, \pi; \mathbf{A}, \mathbf{E}] e^{-iD[\varphi, \pi; \mathbf{A}, \mathbf{E}]}
\]
\[
\equiv H [\chi, \pi; \mathbf{W}, \mathbf{E}],
\]
(7.131)
where
\[
\chi (\mathbf{x}) = e^{iD[\varphi, \pi; \mathbf{A}, \mathbf{E}]} \psi (\mathbf{x}) e^{-iD[\varphi, \pi; \mathbf{A}, \mathbf{E}]},
\]
(7.132)
\[
\mathbf{W} (\mathbf{x}) = e^{iD[\varphi, \pi; \mathbf{A}, \mathbf{E}]} \mathbf{A} (\mathbf{x}) e^{-iD[\varphi, \pi; \mathbf{A}, \mathbf{E}]},
\]
(7.133)
As is well known, within the temporal gauge, the electromagnetic field still has gauge degrees of freedom; the Hamiltonian $H [\psi, \pi; \mathbf{A}, \mathbf{E}]$ remains invariant under any time-independent gauge transformation. As another representation of $H [\psi, \pi; \mathbf{A}, \mathbf{E}]$, the Hamiltonian $H [\chi, \pi; \mathbf{W}, \mathbf{E}]$ is also gauge invariant,
\[
H [\chi, \pi; \mathbf{W}, \mathbf{E}] = e^{iG[\theta, \chi, \pi, \mathbf{E}]} H [\chi, \pi; \mathbf{W}, \mathbf{E}] e^{-iG[\theta, \chi, \pi, \mathbf{E}]},
\]
(7.134)
where $\theta \in \mathbb{R}$ and
\[
G [\theta, \chi, \pi, \mathbf{E}] = \int d\mathbf{x} [-ie\theta (\pi\chi - \chi^\dagger \pi^\dagger) + \nabla \theta \cdot \mathbf{E}].
\]
(7.135)
As Higgs [69]–[71] did, we can re-gauge the fields $\chi (\mathbf{x})$ and $\mathbf{W} (\mathbf{x})$ by letting $\theta (\mathbf{x})$ equal the phase of $\chi (\mathbf{x})$; that is,
\[
\chi (\mathbf{x}) = \rho (\mathbf{x}) e^{i\theta (\mathbf{x})}, \quad \rho (\mathbf{x}) \in \mathbb{R},
\]
(7.136)
so as to eliminate the Goldstone bosons represented by the phase of $\chi (\mathbf{x})$. Upon such a choice of $\theta (\mathbf{x})$, the Hamiltonian $H_0$ can be expressed as
\[
H_0 = \int d\mathbf{x} \left[ \hat{\pi}^\dagger \hat{\pi} + (\nabla + ie\hat{\mathbf{A}}) \rho : (\nabla - ie\hat{\mathbf{A}}) \rho + m^2 \rho^2 + g \rho^4 + \frac{1}{2} E^2 + \frac{1}{2} (\nabla \times \hat{\mathbf{A}})^2 \right],
\]
(7.137)
where
\[
\hat{\pi} (\mathbf{x}) = e^{iG[\theta, \chi, \pi, \mathbf{E}]} \pi (\mathbf{x}) e^{-iG[\theta, \chi, \pi, \mathbf{E}]},
\]
(7.138)
\[
\hat{\mathbf{A}} (\mathbf{x}) = e^{iG[\theta, \chi, \pi, \mathbf{E}]} \mathbf{W} (\mathbf{x}) e^{-iG[\theta, \chi, \pi, \mathbf{E}]},
\]
(7.139)
From equations (7.132) and (7.121), it follows that
\[ \chi(x) = \psi(x) + \varphi(x). \]  
(7.140)

Without loss of generality, we can, from equation (7.128), choose \( \varphi(x) \) as real,
\[ \varphi(x) = \nu / \sqrt{2}. \]  
(7.141)

That leads to
\[ \rho(x) = (\phi(x) + \nu) / \sqrt{2}, \]  
where
\[ \phi(x) = \sqrt{2} e^{iG[\theta, \tilde{\psi}, \pi, E]} \psi(x) e^{-iG[\theta, \tilde{\psi}, \pi, E]}. \]  
(7.143)

Equation (7.142) indicates that \( \phi(x) \) is merely a real field.

Substitution of equation (7.142) into equation (7.137) gives rise to
\[ H_0 = \int dx \left[ \frac{1}{2} p^2 + \frac{1}{2} \left( \nabla + ie\tilde{A} \right) \phi \cdot (\nabla - ie\tilde{A}) \phi - m^2 \phi^2 + g\nu \phi^3 + \frac{g}{4} \phi^4 
+ \frac{1}{2} E^2 + \frac{1}{2} (\nabla \times \tilde{A})^2 + \frac{1}{2} e^2 \nu^2 \tilde{A} \cdot \tilde{A} + e^2 \nu \phi \tilde{A} \cdot \tilde{A} - \frac{g\nu^4}{4} + \frac{1}{2} p_0^2 \right], \]  
(7.144)

where
\[ p(x) = \left[ \tilde{\pi}^\dagger(x) + \tilde{\pi}(x) \right] / \sqrt{2}, \]  
(7.145)
\[ p_0(x) = i[\tilde{\pi}^\dagger(x) - \tilde{\pi}(x)] / \sqrt{2}. \]  
(7.146)

Paying attention to
\[ e^{iG[\theta, \chi, \pi, E]} \left( \frac{\chi(x) + \chi^\dagger(x)}{\sqrt{2}} \right) e^{-iG[\theta, \chi, \pi, E]} = \phi(x) + \nu, \]  
(7.147)

we have
\[ [p(x), \phi(x')] = -i \delta(x - x'), \]  
(7.148)
\[ [p_0(x), H_0] = 0. \]  
(7.149)

That is to say, \( \phi(x) \) and \( p(x) \) become a new pair of canonical field operators, whereas \( p_0(x) \) is just a constant. Physically, that is because \( p_0(x) \) corresponds to the eliminated degree of freedom \( \phi_0(x) = -i \left( \chi(x) - \chi^\dagger(x) \right) / \sqrt{2} \).

Equation (7.144) forms the Higgs picture of creation of mass. Comparing it with equation (7.129), one sees immediately that the mass of the gauge field in Higgs picture is identical to that in Ginzburg–Landau picture, as is expected.

The above theory for a complex field coupled with an Abelian gauge field can be easily generalized to the case of an \( N \)-component field coupled with a non-Abelian gauge field, with the same conclusion that the gauge field will obtain a mass through spontaneous symmetry breaking. This manner of mass producing is the well-known Higgs mechanism, which was successively contributed to by London [68], Ginzburg and Landau [51], Anderson [72, 73], Higgs [69]–[71], and Kibble [74].

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Remark. Spontaneous symmetry breaking can occur without any fundamental Higgs field in superconductivity; it is thus called ‘dynamical symmetry breaking’, which implies that Higgs fields are ‘normally’ needed for symmetry breaking. From the viewpoint of the extended ensemble theory, that is a prejudice because superconductivity, Goldstone bosons and Higgs mechanism share the same physical ground. This is in accordance with the standpoint of Huang expressed in his book [75].

8. Summary and conclusions

A possible extension of Gibbs ensemble theory has been postulated, as a personal review of the author, to enable a microscopic description to phase transitions and spontaneous symmetry breaking. The extension is founded on three hypotheses, which root, in physics, from Landau’s ideas on phase transitions, i.e., order parameter, variational principle, representation transformation, and spontaneous symmetry breaking. In this sense, the extended Gibbs ensemble theory can be viewed as a microscopic realization of the Landau phenomenological theory of phase transitions.

Within the framework of the extended ensemble theory, a phase transition occurs according to the principle of least entropy, which manifests itself as an equation of motion of the order parameter. This equation determines the evolution of the order parameter with temperature, and thus controls the change in representation of the system Hamiltonian. Different phases correspond to different representations, and vice versa. A system Hamiltonian will realize its symmetric representation in the disordered phase, and its asymmetric one in the ordered phase. The change in symmetry results from the change in representation. That is the Landau mechanism in the extended ensemble theory; it accounts for phase transitions and spontaneous symmetry breaking, and holds in the whole range of temperature, including the critical region.

Physically, phase transitions originate from the wave nature of matter. A system always stays in its normal phase at sufficiently high temperatures, which is disordered and structureless. As the temperature decreases, matter waves will interfere automatically with one another. This interference makes the system to be structured and to transform into its ordered phase. That is the physical picture for phase transitions in the extended ensemble theory.

Also, the extended ensemble theory has been applied to typical quantum many-body systems, with the conclusions as follows.

The ideal Fermi gas cannot produce superconductivity; its normal phase is stable at any temperature.

Negative-temperature and laser phases arise from the same mechanism as phase transitions; they are both unstable, and will finally turn into the positive-temperature phase. That is the microscopic interpretation for negative temperatures and laser phases.

For the conventional weak-coupling low-$T_c$ superconductors, the mean-field solution due to Bardeen, Cooper and Schrieffer is derived anew, and is proved to be stable within the extended ensemble theory.

The ideal Bose gas can produce Bose–Einstein condensation only in the thermodynamic limit, which agrees with Einstein’s prediction. But that holds in the sense of Lebesgue integration rather than Riemann integration. In general, the order
Extended ensemble theory, spontaneous symmetry breaking, and phase transitions

parameter for BEC cannot be interpreted as the number of condensed particles. Besides, there cannot exist any supercurrent or vortex in the ideal Bose gas; the condensation is always homogeneous.

The ideal phonon gas cannot produce Bose–Einstein condensation; neither can the photon gas in a black body.

It is not admissible to quantize the Dirac field using Bose–Einstein statistics. Otherwise, the system is unstable. That is a statistical rather than mechanical reason why the Dirac field has to be quantized using Fermi–Dirac statistics. This conclusion is in accordance with the spin-statistics theorem in quantum field theory.

A structural phase transition belongs physically to the Bose–Einstein condensation occurring in configuration space. A double-well anharmonic system is unstable at low temperatures, and will undergo a structural phase transition at a finite temperature. Physically, that is because the position fluctuation is a monotonically decreasing function of temperature.

For the $O(N)$-symmetric vector model, the $O(N)$ symmetry will break down spontaneously, with the presence of Goldstone bosons. In essence, this SSB is a Bose–Einstein condensation. If the system is coupled with a gauge field, it can cause the latter to condense together with itself. The cooperative condensation can be described by Ginzburg–Landau equations. After the condensation, the gauge field can obtain a mass, which is the so-called Higgs mechanism.

An interacting Bose gas is stable only if the interaction is repulsive. The BEC present in this system can be described by the generalized Ginzburg–Landau equation. If the interaction is weak, the BEC is a ‘$\lambda$-transition’, and its transition temperature can be lowered by the repulsive interaction. As a characteristic property of this ‘$\lambda$-transition’, the specific heat at constant volume $C_V$ will vanish linearly as $T \to 0$.

If liquid $^4$He could be regarded as a weakly interacting Bose gas, and if the $\lambda$-transition were a Bose–Einstein condensation, then its specific heat at constant pressure $C_P$ would show a $T^3$ law at low temperatures, which is in agreement with the experiment. However, if temperature goes lower, it is predicted that $C_P$ will exhibit a linear behaviour at relatively lower temperatures, which is in need of experimental verifications.

Acknowledgments

The author would like to thank Professor Zheng-zhong Li, Professor Jin-ming Dong, and Professor Wei-yi Zhang for their helpful discussions. He is also deeply grateful to Professor Vladimir Rittenberg for his valuable advice on how to revise the paper.

Appendix A. Frequency summation

In this appendix, we shall first show that, when $\mu > 0$, the ideal Bose gas is still well defined within the extended ensemble theory, and then discuss the frequency summation, which is very useful when we attempt to solve problems through Green’s functions.

Upon a transformation as in equation (3.2), the statistical average defined by equation (2.3) can always be transformed into a statistical average with respect to the Hamiltonian $H(b)$ of equation (5.1). It is thus sufficient for us to show that the statistical average with respect to $H(b)$ is properly defined when $\mu > 0$. As is well known, every statistical average can be calculated through a corresponding Green’s function, and every
Green’s function can be derived from the generating functional of the system. Therefore, we need only to prove that the generating functional is properly defined when $\mu > 0$.

According to the path-integral formalism [76], the generating functional $W[\phi^+, \phi]$ for $H(b)$ can be written as follows:

$$
W[\phi^+, \phi] = \mathcal{N}^{-1} \int \mathcal{D}b^+ \mathcal{D}b \exp \left( \frac{1}{\hbar} \sum_{k,n} \left( b_{k,n}^+ \left[ i\hbar \omega_n - \left( \frac{\hbar^2 k^2}{2m} - \mu \right) \right] b_{k,n} - \phi_{k,n} b_{k,n}^+ - \phi_{k,n}^+ b_{k,n} \right) \right), \tag{A.1}
$$

where $\omega_n = 2n\pi/\beta$ ($n \in \mathbb{Z}$) denotes the Matsubara frequency, and $\mathcal{N}$ the normalization factor,

$$
\mathcal{N} = \int \mathcal{D}b^+ \mathcal{D}b \exp \left( \frac{1}{\hbar} \sum_{k,n} b_{k,n}^+ \left[ i\hbar \omega_n - \left( \frac{\hbar^2 k^2}{2m} - \mu \right) b_{k,n} \right] \right). \tag{A.2}
$$

If $\mu < 0$, one gets immediately the familiar result,

$$
W[\phi^+, \phi] = \exp \left( -\frac{1}{\hbar} \sum_{k,n} \phi_{k,n} b_{k,n}^+ \frac{1}{i\hbar \omega_n - ((\hbar^2 k^2/2m) - \mu) \phi_{k,n}^+} \right). \tag{A.3}
$$

Since $\hbar^2 k^2/(2m) - \mu > 0$, the normalization factor $\mathcal{N}$ converges.

When $\mu \geq 0$, the normalization factor $\mathcal{N}$ will diverge. However, that does no harm because the normalization factor can be cancelled by the numerator of equation (A.1), as is frequently encountered in quantum field theory [49]. After the cancellation, the rest is still equation (A.3) except $\mu \geq 0$. As mentioned in section 5, an unbounded function as integrand is permissible within Lebesgue integration. Therefore, the sum in the exponent of equation (A.3) is proper as a Lebesgue integral. The resulting $W[\phi^+, \phi]$ is also acceptable because a function is permitted to be unbounded in Lebesgue integration.

In a word, the generating functional for $H(b)$ is always properly defined no matter how large the chemical potential $\mu$ is, which ends our proof.

Now, there is no mathematical limit on the chemical potential of the ideal Bose gas, as is the case for the ideal Fermi gas. That is rational and significant: any limit on chemical potential should be set by the physical theory itself rather than by the mathematical theory involved. In the extended ensemble theory, the chemical potential of a system is determined only by the physical requirement: the conservation of particles, whether the system obeys Bose–Einstein statistics or Fermi–Dirac statistics; there is no limit set by the mathematical tool, i.e., Lebesgue integration.

As a consequence of equation (A.3), we obtain

$$
G(k, i\omega_n) = -\left( -\frac{1}{\hbar} \right)^{-2} \frac{\delta^2 W[\phi^+, \phi]}{\delta \phi_{k,n}^+ \delta \phi_{k,n}} = \frac{1}{i\omega_n - \hbar^{-1} ((\hbar^2 k^2/2m) - \mu)}, \tag{A.4}
$$

where $G(k, i\omega_n)$ represents the temperature Green’s function which is defined as [54]

$$
G(k, \tau - \tau') = -\text{Tr} \left( T_\tau \{ b_k(\tau)b_k^+(\tau') \} \rho(H(b)) \right). \tag{A.5}
$$
As a function of $k$, $G(k, i\omega_n)$ can be unbounded if $\mu \geq 0$, but that will be all right because $G(k, i\omega_n)$ can only appear in the integrand of a Lebesgue integral over $k$.

Those discussions indicate that, in the manipulations of $+\infty$ and $-\infty$, one can benefit greatly from Lebesgue integration. That is because Lebesgue integration is designed, ab initio, on the set of extended real numbers: $\mathbb{R}^3 = \mathbb{R} \cup \{+\infty\} \cup \{-\infty\}$ where $\mathbb{R} = (-\infty, +\infty)$ [42]. Evidently, those benefits cannot be provided by Riemann integration. More benefits of Lebesgue integration will be seen from the following discussions.

When one evaluates the statistical average of an observable, one will encounter the summation over Mutohsara frequencies. As an illustration, let us consider discussions. Integration. More benefits of Lebesgue integration will be seen from the following.

To perform the frequency summation, it is helpful to make use of the complex function, which has simple poles at the Mutohsara frequencies, i.e., $z = i\omega_n = i2n\pi/\beta\hbar$, and transform the summation into a contour integral [54],

$$
\left(\frac{1}{\beta\hbar}\right)\sum_n e^{i\eta z}G(k, i\omega_n) = \int_C \frac{dz}{2\pi i} e^{inz} f(z)G(k, z),
$$

where the contour $C$ is depicted in figure A.1. It should be emphasized that the above procedure requires that the function $G(k, z)$ must be analytic on the whole imaginary axis lest there be any poles other than $\omega_n$ on this axis. Sometimes, this requirement cannot be met by every $k$, e.g.,

$$
G(k, z) = \frac{1}{z - \hbar^{-1}(\hbar^2 k^2/2m) - \mu}, \quad \mu \geq 0.
$$

Each such $G(k, z)$ that satisfies $|k| = \sqrt{2m\mu}/\hbar$ is singular on $z = 0$, and thus cannot meet the requirement. If such singular $k$ constitute just a null set $D$, i.e., $G(k, z)$ satisfies the requirement almost everywhere on $\mathbb{R}^3$, which is the usual case, then those $k$ can be left out of consideration for they give merely a null contribution to the Lebesgue integral over $k$. Therefore, we can rewrite equation (A.6) as

$$
\int_{\mathbb{R}^3} dk \left(\frac{1}{\beta\hbar}\right)\sum_n e^{i\eta z}G(k, i\omega_n) = \int_E \frac{dz}{C} \frac{dz}{2\pi i} e^{inz} f(z)G(k, z),
$$

where $E = \mathbb{R}^3 \setminus D$. Here the set $D$ is removed form $\mathbb{R}^3$ so that the function $G(k, z)$ can meet the requirement everywhere on $E$.

Generally, $G(k, z)$ are analytic on both the upper and lower half complex-$z$ planes [39, 54], and one can therefore deform the contour $C$ into the contours $\Gamma$ and $C'$, which results in

$$
\int_C \frac{dz}{2\pi i} e^{inz} f(z)G(k, z) = \int_{C'} \frac{dz}{2\pi i} f(z)G(k, z).
$$
Figure A.1. The counters for the frequency summation of a Bose system.

The contribution from the contour $\Gamma$ vanishes owing to the convergence factor $e^{i\eta z}$ [54]. The right-hand side can be simplified as

$$\int_{C'} \frac{dz}{2\pi i} f(z)G(k, z) = \mathcal{P} \int_{-\infty}^{+\infty} d\omega f(\omega)A(k, \omega),$$

(A.12)

where $A(k, \omega)$ is the spectral intensity,

$$A(k, \omega) = -\frac{1}{2\pi i} \left[ G(k, \omega + i0^+) - G(k, \omega - i0^+) \right],$$

(A.13)

and $\mathcal{P}$ represents the principal value,

$$\mathcal{P} \int_{-\infty}^{+\infty} d\omega f(\omega)G(k, \omega) = \lim_{\alpha \to 0^+} \left( \int_{-\infty}^{-\alpha} d\omega f(\omega)A(k, \omega) + \int_{\alpha}^{+\infty} d\omega f(\omega)A(k, \omega) \right).$$

(A.14)

Substituting equations (A.11)–(A.14) into equation (A.10), one has

$$\int_{\mathbb{R}^3} dk \left(-\frac{1}{\beta \hbar}\right) \sum_n e^{i\omega_n \eta} G(k, i\omega_n)$$

$$= \int_{E} dk \lim_{\alpha \to -0^+} \left[ \int_{-\infty}^{-\alpha} d\omega f(\omega)A(k, \omega) + \int_{\alpha}^{+\infty} d\omega f(\omega)A(k, \omega) \right]$$

$$= \lim_{\alpha \to -0^+} \int_{E} dk \left[ \int_{-\infty}^{-\alpha} d\omega f(\omega)A(k, \omega) + \int_{\alpha}^{+\infty} d\omega f(\omega)A(k, \omega) \right]$$

$$= \lim_{\alpha \to -0^+} \left[ \int_{-\infty}^{-\alpha} d\omega f(\omega) \int_{E} dk A(k, \omega) + \int_{\alpha}^{+\infty} d\omega f(\omega) \int_{E} dk A(k, \omega) \right]$$

$$= \mathcal{P} \int_{-\infty}^{+\infty} d\omega f(\omega) \int_{E} dk A(k, \omega).$$

(A.15)
Now, supplementing the set $E$ with the null set $D$, one arrives at
\[
\int_{\mathbb{R}^3} dk \left( \frac{1}{\beta \hbar} \right) \sum_n e^{i\omega_n \eta} G(k, i\omega_n) = \mathcal{P} \int_{-\infty}^{+\infty} d\omega f(\omega) \int_{\mathbb{R}^3} dk A(k, \omega). \tag{A.16}
\]

As usual, by introducing the density of states $N(\omega)$,
\[
N(\omega) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} dk A(k, \omega). \tag{A.17}
\]

Equation (A.16) can be reduced into
\[
\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} dk \left( \frac{1}{\beta \hbar} \right) \sum_n e^{i\omega_n \eta} G(k, i\omega_n) = \mathcal{P} \int_{-\infty}^{+\infty} d\omega \frac{N(\omega)}{e^{\beta \hbar \omega} - 1}. \tag{A.18}
\]

This is a very useful identity; for example, one can easily obtain the final results of equations (5.36) and (5.39) with this identity. It should be stressed that equation (A.18) holds whether the chemical potential $\mu$ is less than, equal to, or larger than zero. If $\mu < 0$, it reduces to the common result given in [54]. It is a generalization of the common result when $\mu \geq 0$. This generalization removes the mathematical limit on the chemical potential. One cannot reach the result of equation (A.18) within Riemann integration.

Obviously, the above analyses for the ideal Bose gas are also suitable for other Bose systems, e.g., the interacting Bose gas, which is studied in section 7.1.

**Remark 5.** If the system obeys Fermi–Dirac statistics, the principal value is unnecessary. Instead of equation (A.18), one has
\[
\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} dk \left( \frac{1}{\beta \hbar} \right) \sum_n e^{i\omega_n \eta} G(k, i\omega_n) = \mathcal{P} \int_{-\infty}^{+\infty} d\omega \frac{N(\omega)}{e^{\beta \hbar \omega} + 1} = \int_{-\infty}^{+\infty} d\omega \frac{N(\omega)}{e^{\beta \hbar \omega} + 1}. \tag{A.19}
\]

That is simply because the Fermi distribution function is bounded and continuous at $\omega = 0$ for any finite temperature $\beta > 0$. A more direct reason for the unrechness of the
principal value consists in the fact that, unlike the Bose system, $z = 0$ is not the pole of the complex function,

$$f(z) = \frac{1}{e^{\beta \omega} + 1}, \quad (A.20)$$

because the Matsubara frequencies for a Fermi system are all nonzero, i.e., $\omega_n = (2n + 1) \pi/\beta \hbar \neq 0$ ($n \in \mathbb{Z}$). As a consequence, the integration contour can go as in figure A.2, which gives straightforwardly the final result of equation (A.19). Evidently, that makes the Fermi system easier to handle mathematically than the Bose system.

### Appendix B. Low-temperature thermal activations of a weakly interacting Bose system

In section 7.1, our discussions were confined within the Hartree–Fock approximation of equations (7.12)–(7.13) and the short-range approximation of equation (7.22). Within those approximations, one sees from equations (7.40) and (7.44) that the thermal activations at low temperatures can be expanded into even power series of $T$. We shall show that, beyond those approximations, this feature still holds as long as the interaction is weak and perturbative.

Under the condition assumed, observables can be calculated via GFs. The calculations can be transformed finally into the integrals of the following form:

$$\mathcal{P} \int_{-\infty}^{+\infty} d\omega \frac{g(\omega, \tilde{\mu})}{e^{\beta \omega} - 1}, \quad (B.1)$$

where $g(\omega, \tilde{\mu})$ is a real-valued function of $\omega$ and $\tilde{\mu}$, which comes from the summation of a corresponding GF over $k$. As a function of $\omega$, $g(\omega, \tilde{\mu})$ should be bounded at bottom or decrease quickly with $\omega$ so that the integral can converge. In both cases, we can cut off the integral from below at a certain frequency $-\omega_c$ ($\omega_c > 0$), that is,

$$\mathcal{P} \int_{-\infty}^{+\infty} d\omega \frac{g(\omega, \tilde{\mu})}{e^{\beta \omega} - 1} = \mathcal{P} \int_{-\omega_c}^{+\infty} d\omega \frac{g(\omega, \tilde{\mu})}{e^{\beta \omega} - 1}. \quad (B.2)$$

According to the definition of principal value, the right-hand side can be written as

$$\mathcal{P} \int_{-\omega_c}^{+\infty} d\omega \frac{g(\omega, \tilde{\mu})}{e^{\beta \omega} - 1} = \int_{-\omega_c}^{0} d\omega \frac{g(\omega, \tilde{\mu})}{e^{\beta \omega} - 1} + \int_{0}^{+\infty} d\omega \frac{g(\omega, \tilde{\mu})}{e^{\beta \omega} - 1}. \quad (B.3)$$

Observe that

$$\frac{1}{e^{\beta \omega} - 1} + \frac{1}{e^{-\beta \omega} - 1} = -1; \quad (B.4)$$

we have

$$\mathcal{P} \int_{-\infty}^{+\infty} d\omega \frac{g(\omega, \tilde{\mu})}{e^{\beta \omega} - 1} = - \int_{-\omega_c}^{0} d\omega \frac{g(\omega, \tilde{\mu})}{e^{\beta \omega} - 1} - \int_{-\omega_c}^{0} d\omega \frac{g(\omega, \tilde{\mu})}{e^{-\beta \omega} - 1} + \int_{0}^{+\infty} d\omega \frac{g(\omega, \tilde{\mu})}{e^{\beta \omega} - 1}. \quad (B.5)$$
Integrated by substitution, this turns into
\[
P \int_{-\infty}^{+\infty} d\omega \frac{g(\omega, \bar{\mu})}{e^{\beta\omega} - 1} = - \int_{0}^{\omega_c} d\omega g(\omega - \omega_c, \bar{\mu}) + k_B T \int_{0}^{+\infty} dx \frac{g(\omega_c + k_B Tx, \bar{\mu})}{e^{x} - 1} + k_B T \int_{0}^{\omega_c} dx \frac{g(k_B Tx, \bar{\mu}) - g(-k_B Tx, \bar{\mu})}{e^{x} - 1}.
\] (B.6)

The second integral on the right-hand side vanishes exponentially as \(T \to 0\); it can thus be neglected. The upper limit of the third integral can be set equal to \(+\infty\) at low temperatures for the integrand decreases as \(e^{-x}\) when \(x\) becomes very large,
\[
P \int_{-\infty}^{+\infty} d\omega \frac{g(\omega, \bar{\mu})}{e^{\beta\omega} - 1} = - \int_{0}^{\omega_c} d\omega g(\omega - \omega_c, \bar{\mu}) + k_B T \int_{0}^{+\infty} dx \frac{g(k_B Tx, \bar{\mu}) - g(-k_B Tx, \bar{\mu})}{e^{x} - 1}.
\] (B.7)

The second integral on the right-hand side can expanded as
\[
\int_{0}^{+\infty} dx \frac{g(k_B Tx, \bar{\mu}) - g(-k_B Tx, \bar{\mu})}{e^{x} - 1} = 2 \sum_{n=1}^{+\infty} \zeta(2n)g^{(2n-1)}(0, \bar{\mu})(k_B T)^{2n-1}.
\] (B.8)

Substituting it into equation (B.7) results in
\[
P \int_{-\infty}^{+\infty} d\omega \frac{g(\omega, \bar{\mu})}{e^{\beta\omega} - 1} = - \int_{0}^{\omega_c} d\omega g(\omega - \omega_c, \bar{\mu}) + 2 \sum_{n=1}^{+\infty} \zeta(2n)g^{(2n-1)}(0, \bar{\mu})(k_B T)^{2n};
\] (B.9)

the sum is an even power series of \(T\). To the fourth order, it becomes
\[
P \int_{-\infty}^{+\infty} d\omega \frac{g(\omega, \bar{\mu})}{e^{\beta\omega} - 1} = - \int_{0}^{\omega_c} d\omega g(\omega - \omega_c, \bar{\mu}) + 2\zeta(2)g'(0, \bar{\mu})(k_B T)^2 + 2\zeta(4)g^{(3)}(0, \bar{\mu})(k_B T)^4;
\] (B.10)

which is sufficient for the discussion of the low-temperature properties of the system. This result implies that the renormalized chemical potential \(\bar{\mu}\) and the internal energy \(E\) are even functions of \(T\) at low temperatures, which leads to the conclusion of equation (7.45): the specific heat \(C_V\) of a weakly interacting Bose gas will vanish linearly as \(T \to 0\).

The above result reminds us of the specific heat of the electron gas in a normal metal, which also vanishes linearly as \(T \to 0\). This linear behaviour of the electron gas can be explained analogously. There, what is concerned is the integral,
\[
\int_{-\infty}^{+\infty} d\omega \frac{g(\omega, \mu)}{e^{\beta\omega} + 1};
\] (B.11)

where \(\mu\) is the chemical potential. In the same way as for the Bose gas, it can be expressed as
\[
\int_{-\infty}^{+\infty} d\omega \frac{g(\omega, \mu)}{e^{\beta\omega} + 1} = \int_{0}^{\omega_c} d\omega g(\omega - \omega_c, \mu) + 2 \sum_{n=1}^{+\infty} \left(1 - \frac{1}{2^{2n-1}}\right) \zeta(2n)g^{(2n-1)}(0, \mu)(k_B T)^{2n}.
\] (B.12)
To the second order, it is
\[
\int_{-\infty}^{+\infty} d\omega \frac{g(\omega, \mu)}{e^{\beta \omega} + 1} = \int_{0}^{\omega_c} d\omega g(\omega - \omega_c, \mu) + \zeta(2)g'(0, \mu)(k_B T)^2 , \tag{B.13}
\]
which is sufficient for the low-temperature properties of the electron gas in a normal metal because its Fermi temperature is very high, in comparison to the critical temperature of the BEC happening in a weakly interacting Bose gas. Equation (B.13) also implies that the chemical potential $\mu$ and the internal energy $E$ are even functions of $T$ at low temperatures, and that the specific heat at constant volume $C_V$ will vanish linearly as $T \to 0$. For example, one can easily verify, with the help of equation (B.13), that the $\mu$, $E$ and $C_V$ for the ideal Fermi gas have the low-temperature forms

\[
\mu(T) = \mu(0) \left[ 1 - \frac{\pi^2}{12} \left( \frac{k_B T}{\mu(0)} \right)^2 \right], \tag{B.14}
\]

\[
\frac{E}{N} = \frac{3}{5} \mu(0) \left[ 1 + \frac{5\pi^2}{12} \left( \frac{k_B T}{\mu(0)} \right)^2 \right], \quad \frac{C_V}{Nk_B} = \frac{\pi^2}{2} \frac{k_B T}{\mu(0)}. \tag{B.15}
\]

which are familiar results. These discussions show that similarity exists even between such different systems!

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