A new set of quasi-particle operators are introduced into the theory of a degenerate system of bosons in which the depletion of the condensate is appreciable. These operators are related by a nonlinear canonical transformation to the density fluctuation operators and their canonical conjugates. The quasi-particles have a temperature dependent phonon spectrum. They incorporate the interaction between bosons with non-zero momenta. In the limit as the density of the condensate approaches zero, the proposed theory is reduced to the Hartree-Fock theory for a nondegenerate system.

In a series of papers the present author and his collaborators have developed a theory of a degenerate system of weakly interacting bosons at zero temperature using collective variables. With the aid of a nonlinear canonical transformation which relates these variables to the operators describing approximate quasi-particles, it has been possible to derive the phonon-type excitation spectrum avoiding infrared and ultraviolet divergences. Here, we extend the theory to finite temperatures by taking into consideration the depletion of the zero-momentum condensate caused by thermal excitations.

The fundamental collective variables are the density fluctuation operators \( \varphi_k \) and their canonical conjugates \( \varphi^*_{-k} \). These can be written in terms of the boson creation and annihilation operators \( a_p \) as

\[
\varphi_k = \sum_p a_p \varphi_{p+k},
\]

\[
\varphi_k = \varphi_k^{(t)} + \varphi_k^{(u)^*},
\]

and

\[
\varphi_k^{(t)} = (i\hbar/2) \sum_{f=1}^m (-1)^{f-1} \times \sum_{p_1 \ldots p_f} \delta_{k-p} \prod_{i=1}^f (a_{p_i} a_{p_i}^{-1}),
\]

where the prime on \( \sum \) implies that the summation variables cannot take the value zero, \( \delta_{k-p} = \delta_{k-p} \) is the Kronecker symbol and the inverse operator \( a_0^{-1} \) of \( a_0 \) is given by

\[
a_0^{-1} = \sum_{p_1, \ldots, p_m} \prod_{i=1}^m \left( \frac{1}{N} a_{p_i}^* \right) \frac{1}{N} a_0^* \prod_{i=1}^m a_{p_i}, \quad \mathcal{N} = \rho_0.
\]

The collective variables can be used to rewrite the Hamiltonian

\[
H = \sum_k \frac{\hbar^2 k^2}{2m} a_k^* a_k + \frac{1}{2 \Omega} \sum_{p,q,h} \nu(k) a_p^* a_q + \frac{\hbar^2 p^2}{8 m} + W[\rho] 
\]

\[
+ \frac{1}{2 \Omega} \sum_p \nu(p) U_{p,-p} - \frac{1}{2 \Omega} N^2 \nu(0),
\]

where we can take \( \rho_0 = \mathcal{N} = N \) and

\[
W[\rho] = \frac{\hbar^2}{8 m N} \sum_p \left[ U_{p,-p} - \frac{1}{2 N_{q,r}^2} \delta_{p+q+r} U_{p,q,r} + \frac{1}{3 N_{q,r,s}^2} \delta_{p+q+r+s} U_{p,q,r,s} - \cdots \right],
\]

\[
U_{p,q} = \rho_p \rho_q - \rho_{p+q},
\]

\[
U_{p,q,r} = \rho_p \rho_q \rho_r - \rho_{p+q} \rho_r + 2 \rho_{p+q+r},
\]

\[
U_{p,q,r,s} = U_{p,q,r} + U_{p,q} + U_{q,r} + U_{r,s} + U_{p,q+s} + U_{q,p+r+s} + U_{r,p+q+s} + U_{p,q+r+s} + U_{p,q+r+s}.
\]

Equation (6) gives the basis for an intuitive understanding of the phonon nature of long wave length excitations because \( H \) is a quadratic function of \( k \varphi_k \). As was pointed out in Ref. 4),
however, when we are to express $H$ in terms of creation and annihilation operators of approximate quasi-particles, we have to relate these operators to $\rho_k$ and $\varphi_k$ in a nonlinear way because ultraviolet divergence would arise if otherwise. The quasi-particle operators $b_p$ we shall use here are related to $\rho_k$ and $\varphi_k$ by a nonlinear canonical transformation which is defined by a formal series in powers of $N_0^{-1/2}$, where $N_0$ is the number of zero momentum particles. Use of such a series, instead of the series in powers of $N^{-1/2}$ as was used in Ref. 4), is suggested by Eqs. (2) and (3) which define a series in powers of $a_0^{-1}$. Our equations relating $b_p$ to $\rho_k$ and $\varphi_k$ are given by

$$\rho_k = \sqrt{N_0} \Lambda_k (B_k^* + B_k),$$

$$\varphi_k = \frac{i \hbar}{2N_0 \Lambda_k} (B_k^* - B_k),$$

where $\Lambda_k$ is a variational parameter and

$$B_k = b_k + \frac{1}{4\sqrt{N_0}} \sum_{p,q} \delta_{k+p+q} \sqrt{\Lambda_k \Lambda_p \Lambda_q} \left( b_p b_q^* + 2 b_p^* b_q - b_q b_p^* - b_q^* b_p \right)$$

$$- \frac{1}{N_0 \sum_{p,q,r}} \delta_{k+p+q+r} \sqrt{\Lambda_k \Lambda_p \Lambda_q \Lambda_r} \left[ \frac{1}{6} (b_p b_p^* b_q b_r^* b_q^* b_r - b_p b_p^* b_q b_r) + \frac{D}{2N_0} b_k^* + \frac{1}{2N_0} (A_k - 1) \sum_p A_p b_{k-p} b_{k-p}^* b_p^* b_p \right]$$

$$+ \frac{1}{4N_0} \Lambda_k \sum_p \sum_{p,q} \left( A_{k-p} - 1 \right) \left( b_{k-p}^* b_{k-p} - b_{k-p} b_{k-p}^* \right) b_k + \ldots.$$  (13)

Equation (13) gives a canonical transformation from $B_k$ to $b_k$ up to the second order terms in $N_0^{-1/2}$. It involves another parameter $D$ to be determined later.

We shall discuss an approximation $\mathcal{S}$ to the free energy of the boson system by considering the grand canonical ensemble of the quasi-particles whose population $J_p$ is treated as a variational parameter. Thus

$$\mathcal{S} = \mathcal{E} - k_b T \sum_p \left[ (\pi_p + 1) \log(\pi_p + 1) - \pi_p \log \pi_p \right],$$

where $\mathcal{E} = \langle H \rangle$ is the expectation value of $H$ in our ensemble at temperature $T$, and $k_b$ is the Boltzmann constant. The optimum value of $\pi_p$ corresponding to the minimum of $\mathcal{S}$ satisfies

$$\pi_p = (e^{\beta p} - 1)^{-1},$$

where $\beta = (k_b T)^{-1}$ and

$$\beta_p = \left( \frac{\delta E}{\delta \pi_p} \right)_{\lambda, N_0}.$$  (16)

The expectation value $\mathcal{E}$ is obtained from the Hamiltonian $H$ which can be expressed in terms of $b_p$ as a series in powers of $N_0^{-1/2}$ using Eqs. (6) through (13). The denominator $N$ in Eq. (7) is also expanded for $N$ around $N_0$. We shall be content with the approximation which is consistent with the terms given explicitly in Eq. (13). Thus the expectation values of the first three terms in Eq. (6) are evaluated by keeping the correction terms which are higher by a factor $N_0^{-1}$ than the leading order contributions. In this way we are lead to

$$\mathcal{E} = \sum_p \left[ \frac{h^2 p^2}{2m} \frac{(A_p - 1)^2}{4A_p} + \frac{A_p^2 + 1}{2A_p} \pi_p^2 \right] - \frac{h^2}{16mN_0} \sum_p \sum_{q,r} \delta_{p+q+r} p^2 (A_p - 1)(A_q - 1)(A_r - 1)$$

$$+ \frac{h^2}{8mN_0} \sum_p \sum_{q,r} (2q^2 A_q - p^2) (A_r - 1) + \frac{q^2}{A_q} (A_q^2 - 1) \right] (A_q - 1)(A_p - 1)$$

$$+ \frac{2p^2 q}{8mN_0} \sum_p \sum_{q,r} \left( A_p^2 - 1 \right) (A_p - 1)(A_q - 1)(A_r - 1)$$

$$+ 2p \cdot q \left( (A_p - 1)(A_q - 1) - (A_p A_q - 1)(A_r - 1) \right) \pi_p \pi_q.$$
Note that for the last expression to be convergent it is necessary that $A_k$ approaches unity in the limit of large $k$

$$\lim_{{k \to \infty}} A_k = 1.$$  \hfill (18)

In the same limit the expectation value $\langle \rho_k \rho_{-k} \rangle$ must approach $N$.

As the limiting value of $\langle \rho_k \rho_{-k} \rangle$ comes out to be $N_0 + D$ thanks to Eqs. (11), (13) and (18), we have to take

$$D = N - N_0.$$  \hfill (19)

The variational equation for $A_k$ which minimizes $\mathcal{G}$ for given values of $T$ and $N$ is given by

$$+ \frac{h^2 k^2}{4m} \left( \frac{1}{A_k^2} \right) \left( \pi_k + \frac{1}{2} \right) \left( 1 + \frac{1}{N_0} \sum_p A_p \pi_p \right)$$

$$- \frac{h^2}{16mN_0} \sum_{p,q} \delta_{k+p+q} (k^2 + p^2 + q^2) (A_p - 1)(A_q - 1)$$

$$+ \frac{h^2}{8mN_0} \sum_{p,q} \delta_{k+p+q} \left[ 2(k^2 A_k + q^2 A_q - q^2 A_p - p^2 A_p - q^2 A_q - 1) \right] (A_p - 1) \pi_k$$

$$+ \frac{h^2}{8mN_0} \sum_{p,q} \delta_{k+p+q} \left[ 2(k^2 A_k + q^2 A_q - p^2 A_p - q^2 A_q - 1) \right] (A_p - 1) \pi_p$$

$$+ \frac{h^2}{4mN_0} \sum_{p,q} \delta_{k+p+q} \left[ 2(k^2 A_k + q^2 A_q - p^2 A_p - q^2 A_q - 1) \right] (A_p - 1) \pi_p$$

$$+ \frac{h^2}{4mN_0} \sum_{p,q} \delta_{k+p+q} \left[ 2(k^2 A_k + q^2 A_q - p^2 A_p - q^2 A_q - 1) \right] (A_p - 1) \pi_p$$

The excitation energy $\epsilon_k$ is obtained from Eqs. (16) and (17) as

$$\epsilon_k = \frac{h^2 k^2}{4m} \frac{A_k^2 - 1}{A_k} + \frac{h^2}{8mN_0} \sum_{p,q} \delta_{k+p+q} \left[ 2(p^2 A_p - k^2)(A_q - 1) + \frac{p^2}{A_p} (A_p - 1) \right] (A_p - 1)$$

Note that the first term on the left-hand side of Eq. (20) is the only term that has a factor $A_k$ in the denominator. As the term carries a factor $k^2$, we find that $A_k$ is proportional to $k$ for small values of $k$ assuming $\nu(0)$ is finite:

$$A_k \propto k.$$  \hfill (21)

The excitation energy $\epsilon_k$ is obtained from Eqs. (16) and (17) as
\[ + \frac{h^2}{4mN_0} \sum_{p,q} \delta_{k+p+q} \left\{ k^2 \Lambda_p \left[ \frac{1}{\Lambda_k} (A_k - 1)^2 + (A_k^2 - 1)(A_k - 1) \right] \right. \]
\[ + p^2 \Lambda_k \left[ \frac{1}{\Lambda_p} (A_p - 1)^2 + (A_p^2 - 1)(A_p - 1) \right] \]
\[ + \frac{-2k \cdot p}{q} \left[ (A_k A_p - 1)(A_q - 1) - (A_k - 1)(A_p - 1) \right] \]
\[ + \frac{1}{2\Omega} \Lambda_k \sum_{p,q} \delta_{k-p-q} \nu(p) \Lambda_p \left( 2\Lambda_p A_q - A_p - 1 \right) \]
\[ + \nu(p)(A_p A_q - A_p - 1) + \nu(q)(A_q^2 - 1) A_p \pi_p. \]  

Equations (21) and (22) prove the phonon nature of the spectrum \( \varepsilon_k \) for small values of \( k \).

In order to have a closed set of equations for given values of \( T \) and \( N \), we shall supplement Eqs. (15), (20) and (22) with the following one which allows \( N_0 \) to be interpreted as the number of condensed particles:
\[ N = N_0 + \sum_p \nu(p) \left[ (A_p - 1)^2 + \frac{A_p^2 + 1}{4A_p} \right]. \]  

The last equation implies that the second term on the right-hand side of the equation
\[ a_0 = (N_0 - N_0 - \sum_p a_p^* a_p)^{1/2} \]
\[ = N_0^{1/2} + (2\sqrt{N_0})^{-1} (N - N_0 - \sum_p a_p^* a_p) + \ldots \]  

has a vanishing expectation value in our ensemble. Equation (23) is derived by following the same lines of reasoning as that developed in Ref. 5). It includes only the leading and the next order terms. In the same approximation, the chemical potential \( \mu \) is given by
\[ \mu = \frac{N}{\Omega} \nu(0) + \frac{1}{2\Omega} \sum_p \nu(p) (A_p - 1 + 2A_p \pi_p). \]  

For a weakly interacting system, \( A_k \) is close to unity except for small \( K \) because \( A_k = 1 \) is the solution of Eq. (20) if \( \nu(k) = 0 \). Equation (23) shows then that \( N_0 \approx N \) when \( T = 0 \). Equation (23) also shows that \( N_0 \) must become zero when \( T \) becomes high enough, because the second term on the right-hand side increases indefinitely for increasing value of \( T \).

Note that the solution \( A_p \) of Eq. (20) has a well-defined limit \( A_p \rightarrow 1 \) when \( N_0 \) approaches zero in spite of the fact that we are using Eq. (13) which has terms that diverge when \( N_0 \rightarrow 0 \). This is because every term carrying a factor \( A_p^{-1} \) on the left-hand side of Eq. (20) has a factor \( A_p^{-1} \) or more so that the equation requires \( A_p^{-1} \) to be proportional to small values of \( N_0 \). In the limit \( N_0 \rightarrow 0 \), Eqs. (22), (23) and (25) take the following forms:
\[ \varepsilon_k = \frac{h^2 k^2}{2m} + \frac{1}{\Omega} \sum_p [\nu(0) + \nu(k-p)] \pi_p - \mu, \]  
\[ N = \sum_p \pi_p, \]  
\[ \mu = \frac{1}{\Omega} \sum_p [\nu(0) + \nu(p)] \pi_p. \]  

Equations (26), (27) and (28) show that, in the thermodynamic limit, our theory simplifies to the Hartree-Fock theory when \( N_0 \) becomes zero.

The above discussion does not necessarily imply that our theory describes the second order transition of the boson system from a degenerate state to a non-degenerate one. As the input parameters in our theory are \( N_0 \) and \( T \) rather than \( N \) and \( T \), \( N_0 \) may come out to be a two- or multi-valued function of \( T \) and \( N \). Further study is necessary in order to determine precisely how \( N_0 \) depends on \( T \).