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Particle vs. pair condensation in attractive Bose liquids

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Résumé. — Nous étudions la compétition entre condensation de particules ou de paires dans un liquide de Bose à l’aide d’une fonction d’onde variationnelle du type champ moléculaire. Cette approximation recouvre le modèle de Bogoliubov pour un gaz de Bose faiblement couplé et l’état de paires de Valatin-Butler. Nous considérons d’abord des bosons sans spin, ignorant le fait qu’un tel gaz ne peut que s’effondrer si les forces sont attractives. Nous montrons que l’état de paires n’existe que si l’attraction est assez forte pour lier deux bosons. La limite des faibles densités est traitée exactement. Aux densités plus élevées, nous utilisons un modèle d’interaction séparable, et nous montrons que les paires se dissocient spontanément pour une densité critique \( N_c \) (pour laquelle leur énergie d’ionisation s’annule). Passé ce seuil, il apparaît un condensat de particules habituel.

Pour éviter l’effondrement, nous considérons des bosons avec une structure de spin interne : l’interaction est liante dans certains états, répulsive en moyenne. Prenant comme exemple des particules de spin 1, nous répétons l’analyse précédente, et nous en validons les résultats, tout en maintenant une compressibilité positive. Dans le régime de paires, l’état fondamental est isotrope (paires singulettes). Passé le seuil de dissociation, il apparaît un condensat de particules anisotrope. Nous montrons que ce condensat est polarisé linéairement (dans une direction arbitraire), et non fragmenté. Nous en discutons brièvement les propriétés physiques, et nous suggérons que la transition paires \( \rightarrow \) particules pourrait être du premier ordre.

Abstract. — The competition between particle and pair condensation in Bose liquids is studied using a mean field variational ground state that comprises both the Bogoliubov approximation for weakly interacting Bose gases and the Valatin-Butler pair state. We first consider structureless bosons, disregarding the fact that an attractive gas will necessarily collapse. We show that a pair state occurs only if the attraction is strong enough to bind two bosons together. The limit of low densities is treated exactly. At higher density, we use a separable interaction model and we show that the pairs dissociate at a critical density \( N_c \) (where their ionization gap vanishes). Past that threshold, ordinary particle condensation sets in.

In order to cure collapse, we consider bosons with an internal spin structure: the interaction is binding in some states, repulsive on the average. Taking spin 1 particles as an example, we repeat the previous analysis, and we substantiate its conclusions while retaining a positive compressibility. In the pair regime the ground state is isotropic (singlet pairs). Past the dissociation threshold, an anisotropic one particle condensate appears. We show that it is linearly polarized (in an arbitrary direction), and non fragmented. We discuss briefly its physical properties, and we suggest that the transition from pair to particle condensation might be first order.

1. Introduction. — The theory of repulsive Bose liquids is fairly well established. Their ground state involves condensation of individual particles into a single quantum state. Although a reliable quantitative theory exists only for weakly interacting [1] or dilute [2] systems, the underlying physics is well understood [3]. In contrast, the situation is far more controversial for attractive systems, which raise a number of difficult questions:

(i) First of all, bosons are prone to collapse, since statistics does not prevent overlap of different particles. Only a strong enough short range repulsion will oppose endless increase of the density. Mathematically, the ground state is stable if the pressure and compressibility are both positive,

\[
pV = N\mu - E_0 > 0; \quad \kappa = \frac{N^2}{V} \frac{\partial \mu}{\partial N} > 0 \tag{1}
\]

\((E_0 \text{ and } \mu \text{ are the ground state energy and chemical potential}).\)
(ii) Second, it is no longer clear whether the ground state involves particle or pair condensation. The latter state, similar to a BCS superconductor, was proposed originally by Valatin and Butler [4]. It has been extensively discussed by Imry and Evans [5], and by many others. Such a pair state is physically obvious in at least one limit: a dilute gas in which the pair interaction is attractive enough to produce a bound state (a feature which does not preclude a short range repulsion). Then molecules should form first; at small enough temperature, they might « Bose condense », leading to the above pair state. Whether such a state can persist without collapse is not clear.

(iii) Finally, there might exist a single particle condensate (meaning a δ-function in the particle distribution $n_k$), without the associated phase locking characteristic of superfluidity. Such states have been envisaged in the past. We shall discuss the corresponding fragmentation of the condensate later in our paper. These three questions are actually interdependent: one cannot answer one while ignoring the others.

The issue is not only of academic interest. Besides the traditional Bose liquid, $^4$He, one may consider « transient » bosons, like excitons in a pumped semiconductor. Whether such excitons can undergo Bose condensation is still argued [6]. Putting aside the experimental issue of cooling them faster than their lifetime, one should avoid two pitfalls.

(i) There should not be a spontaneous liquid gas phase transition into an electron-hole plasma, as in Ge, Si, etc.

(ii) Granted that a dilute gas is stable, it should not crystallize into a solid phase, like molecular $\text{H}_2$ or $^4$He under pressure.

If these conditions are met, Bose condensation should occur. In practice, two excitons do bind into a molecular bie exciton: at low enough density, these molecules should be the condensed entities: excitons undergo pair condensation (1). Similar questions might also arise in the context of nuclear physics: should one pair two nucleons, or $\alpha$ particles which may be viewed as bound deutos?

In the present paper, we take the issue again, using a variational approach similar to that introduced earlier in the study of fermion pairing [7]. Such a language is not new; it was introduced by Girardeau and Arnowit [8] back in 1960. Recently, Dörré, Haug and Tran Thoai [9] used it extensively at finite temperature, in order to discuss possible phase diagrams for realistic interactions. Basically, it corresponds to a mean field approximation, which comprises both the Bogoliubov theory of particle condensation and the Valatin-Butler pair model. In section 2, we first consider the usual problem of structureless bosons (spin 0). If the pair interaction is attractive, such a system does collapse. In a first state, we ignore that feature: we fix the density $N$ arbitrarily. We then use our simple model to set up a language, and to extract simple physical ideas with a minimum of mathematical complexity. In the limit of low densities and strong attraction, that model can be solved exactly, translating for boson pairs the formulation used for fermion pairs by Kjeldysh and Kozlov [10]. We thus prove that pair condensation occurs only if the attraction is strong enough to bind two bosons together. At higher densities, an analytic solution is no longer possible; rather than relying on numerical calculation, we explore in detail the crude model of a separable interaction $V(r, r')$. We show that the minimum attraction for pair condensation becomes stronger and stronger as the density increases—put another way, for a given attraction the « bibosons » tend to dissociate due to their overlap. At a critical density $N_c$, the pure pair state becomes unstable and a particle condensate appears.

For such an analysis to really make sense, one must « cure » collapse. The standard solution is to introduce a short range repulsive core in addition to the long range attraction. A number of attempts have been made along those lines. Following the early work of Huang [11], Jodansk [12] and Chemikova [13] included within first order perturbation theory a long range attraction into the usual theory of dilute repulsive Bose liquids. Clearly, such an approach cannot deal with strong attractions; it cannot describe the transition to pair states. Anyway, if an attraction is strong enough to bind a pair, it will very likely produce collapse, until the density is such as to manifest the repulsive core—but then the bound state is gone! Although it is not formally proven, the existence of condensed bound pairs is probably inconsistent with a positive compressibility for a pure scalar interaction. We must look for some other mechanism for saturation of the density.

An alternate possibility is to introduce particles with an internal spin structure: the interaction may be attractive in some « bonding » spin states, while it is repulsive in « antibonding » states. The standard example is the $\text{H}_2$ molecule: the two electrons have spin $1/2$. The interaction is bonding in the singlet $S = 0$, antibonding in the triplet $S = 1$. Two hydrogen atoms can form a singlet molecule; a third H atom will not be singlet with both the previous ones: bonding cannot extend to more than two particles (put another way, there exists no $\text{H}_3$ covalently linked molecule). That simple example illustrates an important feature: saturation may arise from the internal structure of individual particles.
The example of excitons is once again instructive: they are characterized by an electron spin $S_e$ and a hole spin $S_h$. The total spin $S = S_e + S_h$ may be singlet or triplet. If we ignore interband exchange, $S_e$ and $S_h$ are completely decoupled: the singlet and triplet are degenerate. The exciton is then a «double spin 1/2» particle. If we consider two excitons, 1 and 2, they will interact via an electron-electron exchange $S_{e1} \cdot S_{e2}$, as well as an hole-hole exchange $S_{h1} \cdot S_{h2}$. The bieexciton will correspond to a hole singlet $(S_{h1} + S_{h2} = 0)$ and to an electron singlet $(S_{e1} + S_{e2} = 0)$: here again, a third exciton will not bind to the first two. Note that in that case, the hamiltonian has a double rotational invariance, with respect to $S_e$ and $S_h$ independently.

A particle with two spins 1/2 is indeed a boson, albeit unusual. We may also consider the more traditional case of spin 1 bosons. That would correspond to excitons with a very large interband exchange, such that the singlet triplet splitting is larger than the particle interaction. Only the triplet (which is lowest because of Hund’s rule) enters in the argument. For an orbitally even state (bonding), statistics only allows total spins $S = 0$ or 2. Usually, only the singlet state will be bonding: our saturation mechanism also works.

We note that our point about internal spin structures makes no reference to any momentum dependence of the interactions. We may as well work with short range interactions, involving a single length scale. That is far simpler than the ordinary picture of a strong spin repulsion with a long range attraction. Keeping track of momenta in the calculation is then crucial — and usually it cannot be done reliably. Practically, our model for saturation is much simpler to handle.

In section 3, we study in detail the case of spin 1 bosons, for which the algebra is simpler. We construct the pair state at low density, and we show that it is now stable. We calculate the critical density $N_c$ at which the pairs dissociate (due to multipair exchange). Beyond that threshold, a particle condensate sets in. While the pair state is a singlet, invariant under spin rotation, particle condensation necessarily breaks rotational symmetry. We briefly discuss the nature of the condensate, in terms of polarization, fragmentation, etc... We identify the most favourable ground state, out of which the pairs dissociate (due to multipair exchange). Beyond that threshold, a particle condensate sets in.

Bose condensation of spin 1 particles is an interesting problem in itself: classification and stability of the various ground states, broken symmetries, elementary excitations, etc... These points will be examined in another publication [14]. Here our main emphasis is on saturation mechanism: we want to show that a pair state is consistent with a positive compressibility and that it disappears at higher densities. Spin 1 bosons are a tool, not an aim as such.

2. Ground state of a structureless boson liquid. — We consider $N$ point structureless bosons (spin 0) in a volume $V$. They have mass $m$ and they interact via a pair potential $V(r)$. We assume that $V(r)$ is integrable when $r \to 0$ (possibly with a very large short range repulsion), so that its Fourier transform $V_q$ is well defined. The hamiltonian is easily expressed in terms of creation and destruction operators, $a_k^\dagger$, $a_k$:

$$H = \frac{\hbar^2}{2m} \sum_k k^2 a_k^\dagger a_k + \frac{1}{2} \sum_q V_q \rho_q \rho_{-q}$$

$$\rho_q = \sum_k a_k^\dagger a_{k-q}.$$  

We prove it by considering the Hartree ground state $|\psi_{ON}\rangle = \alpha_0^{\\text{N\,e}} |\text{vac}\rangle$.

The corresponding energy $\frac{1}{2} N^2 V_o$ provides an upper bound to the actual ground state energy $E_0(N)$. If $V_o < 0$, the energy is infinitely negative when $N \to \infty$: complete collapse is unavoidable.

In order to describe Bose condensation, we try a simple variational ansatz for the ground state wave function:

$$|\psi_0\rangle = \frac{1}{N!} \exp[\phi a_0^\dagger + \sum_k \lambda_k a_k^\dagger a_{-k}] |\text{vac}\rangle.$$  

The prime on the summation means that we sum over half momentum space excluding $k = 0$, in order to count each pair $(k, -k)$ only once. $N$ is a normalization factor, easily found by expanding the exponential and using the relation $\langle a^\dagger a^\dagger a a \rangle = a^\dagger a^\dagger a a = 1$:

$$N' = e^{\phi/2} \prod_k \frac{1}{1 - |\lambda_k|^2}.$$  

$\phi$ and $\lambda_k$ are the variational parameters, possibly complex. We may distinguish two cases:

(i) $\phi \neq 0$: (4) describes usual Bose condensation of particles in the $k = 0$ state. If $\lambda_k = 0$, it would reduce to

$$|\psi_0\rangle \sim e^{\phi \delta} |\text{vac}\rangle$$  

which is analogous to (3), taking due account of phase locking and concomitant number fluctuations characteristic of superfluidity. Such a particle condensate is the primary ingredient of the ground state, out of which pairs with opposite momenta can be created via the interaction. These virtually excited pairs correspond to the $\lambda_k$ terms in (4), which are forced by the single particle term $\phi$. Note that (4) is nothing but the Bogoliubov ground state wave function, resulting from a mean field approximate treatment of the hamiltonian (1).

(ii) $\phi \equiv 0$: (4) then describes boson pair condensation, analogous to a BCS superconductor, except that fermions are replaced by bosons. Such states, originally proposed by Valatin and Butler [4], were
extensively discussed by Imry and Evans [5]. The corresponding pair amplitude $\lambda_k$ must be determined self consistently.

Expectation values in the state (4) are easily calculated, for instance by expanding the exponential. We find

$$
\langle a_0 \rangle = \phi, \quad x_k = \langle a_k a_{-k} \rangle = \frac{\lambda_k}{1 - |\lambda_k|^2}
$$

$$
\lambda_k = \langle a_k^* a_k \rangle = \frac{|\lambda_k|^2}{1 - |\lambda_k|^2}
$$

(6)

$n_0 = |\phi|^2$ is the occupancy of the single particle condensate (when it exists). The global phase of $\phi$ and $\lambda_k$ is irrelevant (it corresponds to an arbitrary gauge). On the other hand, the relative phase of $\phi$ and $\lambda_k$ is significant : in what follows, we take $\phi = \sqrt{n_0}$ as real and positive, and we leave the phase of $\lambda_k$ open.

The energy of the state (4) is

$$
E_0 = \sum_k \epsilon_k n_k + \frac{1}{2} N^2 V_0 +
+ n_0 \sum_k n_k V_k + \frac{1}{2} \sum_{k'k''} V_{kk'} n_k n_{k''}
+ n_0 \sum_k \text{Re} x_k V_k + \frac{1}{2} \sum_{k'k''} V_{kk'} x_k^* x_{k''}.
$$

(7)

We have set $\hbar^2 k^2 / 2m = \epsilon_k$ and $n_0 + \sum n_k = N$. The first interaction is the Hartree term, independent of the ground state wave function. The second term is the normal Fock exchange, while the last one is the Bogoliubov anomalous term due to phase locking and number fluctuations. The phase of $x_k$ enters (7) only through the cross term $n_0 x_k$. When $n_0 = 0$, it is completely free, reflecting the separate gauge invariance of condensed pairs. If instead $n_0 \neq 0$, the energy will be minimum if $x_k$ is real, such that

$$
\sum_k V_k x_k < 0.
$$

(8)

Quite generally, we may write (using (6)) :

$$
x_k = \pm \sqrt{n_k(n_k + 1)}.
$$

(9)

The sign in (9) depends on $V_k$ (+ for a pure attraction, − for a pure repulsion).

We note that (7) does not contain any Fock or Bogoliubov interaction terms inside the condensate : the expectation value $\langle a_k^* a_k a_0 a_0 \rangle = n_0(n_0 - 1)$ is calculated directly, without resorting to the various contractions used for the other terms. That feature results from our ansatz (4), in which the condensate involves single particles in a unique state $k = 0$. Such a singular distribution near the origin may also be achieved differently, choosing $\phi \equiv 0$ while assuming that $n_k$ has a sharp peak near $k = 0$ : such a peak is supposed to extend over a number of $(k, -k)$ states large compared to 1, but small compared to $N$ : on a macroscopic scale, it looks like a $\delta$-function. The plain distribution $n_k$ would not distinguish between such a fragmented pseudocondensate and the usual condensate described by (4). Let $p \approx 0$ be a typical momentum belonging to that pseudocondensate : the corresponding expectation values are obtained from (6) with $(\lambda_p)^2 \approx 1$

$$
n_p \gg 1, \quad x_p = n_p e^{i\theta_p}
$$

($\theta_p$ is an arbitrary phase). $n_p$ is necessarily large if a significant fraction of particles is to be packed into a number of states $\ll N$. In calculating the corresponding energy, we need not worry about kinetic energy, which vanishes since $p$ is zero on a macroscopic scale. The only difference with (7) is the reappearance of Fock and Bogoliubov terms inside the pseudocondensate. The corresponding correction to the energy is

$$
\Delta E_0 = \frac{1}{2} V_0 \sum_{p,p'} n_p n_{p'}[1 + e^{i\theta_{p'} - \theta_p}]^2.
$$

If $V_0 > 0$, $\Delta E_0$ is always positive : fragmentation of the condensate is energetically unfavourable. The converse would hold if $V_0$ were $< 0$ : but then we know that the gas would necessarily collapse. We conclude that in any physically meaningful situation, a fragmented pseudocondensate never occurs : either there is no condensate at all ($n_0 - 1$), or if there exists one, it is an ordinary single particle condensate of Bogoliubov type, described by (4). In our opinion, the « pair states with Bose Einstein condensation in the $k = 0$ state », described in the literature [15], are unphysical (2).

(2) In discussing the « pseudocondensate » state, we assumed that the latter was fragmented into a number of states $(\rho, -\rho)$ much larger than 1, albeit not macroscopic. An alternate possibility is to assume a single macroscopically occupied pair state, described by the wave function :

$$
|\psi_0\rangle = \frac{1}{N} \exp \left[ \lambda_0 a_0^2 + \sum_{k=0}^{N/2} \lambda_k a_k a_0^* a_k \right] |\text{Vac}\rangle.
$$

Expanding again the exponential, we find that the $k = 0$ state contributes a factor to the norm

$$
\sum_n \left| \frac{\lambda_0}{\lambda_n} \right|^2 (2n)! = \frac{1}{\sqrt{1 - 4 |\lambda_0|^2}}.
$$

The corresponding expectation values are

$$
n_0 = \frac{4 |\lambda_0|^2}{1 - 4 |\lambda_0|^2}, \quad x_0 = \frac{2 \lambda_0}{1 - 4 |\lambda_0|^2},
$$

$$
\langle a_k^* a_k a_0 a_0 \rangle = \frac{4 |\lambda_0|^2 [1 + 8 |\lambda_0|^2]}{1 - 4 |\lambda_0|^2}.
$$

A macroscopic occupancy of the $k = 0$ state requires $|\lambda_0|^2 \approx 1/4$ : the corresponding contribution to the interaction energy is then $3/2 V_0 n_0^2$ exactly as if that condensate were fragmented. Fragmentation makes no difference — except that it reduces fluctuations. Since anyhow these states are unphysical, the discussion is somewhat semantic.
We now proceed to minimize the energy (7) — or rather \((E - \mu N)\), where \(\mu\) is a chemical potential adjusted at the end in such a way as to achieve the right density \(N\). We first minimize with respect to \(x_k\) at constant \(n_0\), and then with respect to \(n_0\). The first step yields

\[
\left[ \xi_k = \epsilon_k - \mu + NV_0 + n_0 V_k + \sum_k V_{kk'} n_{k'} \right] \frac{dn_k}{dx_k} + \frac{1}{2} \left[ n_0 V_k + \sum_k V_{kk'} x_{k'} \right] = 0. \tag{10}
\]

The solution of (9) and (10) is well known. We set

\[
\xi_k = \epsilon_k - \mu + NV_0 + n_0 V_k + \sum_k V_{kk'} n_{k'}.
\]

\[
\Delta_k = n_0 V_k + \sum_k V_{kk'} x_{k'}.
\]

\[
E_k^2 = \xi_k^2 - \Delta_k^2.
\]

The resulting distributions \(n_k\) and \(x_k\) are given by

\[
n_k = \frac{1}{2} \left[ \frac{\xi_k}{E_k} - 1 \right], \quad x_k = -\frac{\Delta_k}{2E_k} \tag{12}
\]

(11) and (12) must be solved self-consistently. As expected from (8), \(x_k\) is negative for a pure repulsion \((V_k > 0)\), positive for a pure attraction \((V_k < 0)\).

The ground state described by (11) and (12) is meaningful only if \(E_k\) is real, i.e. if \(\xi_k > |\Delta_k|\). That guarantees that \((E - \mu N)\), expressed as a function of \(n_k\)

\[
\xi_k n_k + \Delta_k x_k = \xi_k n_k - |\Delta_k| \sqrt{n_k(n_k + 1)}
\]
does possess a minimum. Such a condition is most stringent when \(\xi_k\) is smallest, i.e. for \(k = 0\). The resulting existence criterion, \(|\Delta_0| < \xi_0\), may be written explicitly as

\[
n_0 V_0 + \sum_k V_k x_k \leq NV_0 - \mu + n_0 V_0 + \sum_k V_k n_k. \tag{13}
\]

The quasiparticle energy \(E_0 > 0\) represents the gap in the single particle excitation spectrum. The situation is especially simple when \(n_0 = 0 : 2E_0\) is then the minimum energy needed to break a condensed pair; making use of (8), we can write the condition (13) as

\[
\mu - NV_0 \leq \sum_k V_k(n_k + x_k). \tag{14}
\]

We now minimize \((E - \mu N)\) with respect to \(n_0\). The pair state \(n_0 = 0\) will be stable if

\[
\frac{\partial(E - \mu N)}{\partial n_0} \geq 0. \tag{15}
\]

Since we already minimized with respect to \(n_k\) we retain only the explicit \(n_0\) dependence in (7) : the condition (15) is then identical to (14). We conclude that a pure pair state will be stable if it possesses a finite positive gap \(E_0\). Viewed in reverse, the pair state ceases to exist when the gap closes to zero : that threshold also marks the spontaneous appearance of a particle condensate, \(n_0 \neq 0\). Past the threshold, \(n_0\) is obtained by minimizing \((E - \mu N)\), according to

\[
\frac{\partial(E - \mu N)}{\partial n_0} = NV_0 - \mu + \sum_k V_k(n_k + x_k) = 0.
\]

In that case, one can eliminate \(\mu\) completely by writing

\[
\xi_k = \epsilon_k + n_0 V_k + \sum_k [V_{kk'} n_{k'} - V_k(n_k + x_k)]. \tag{17}
\]

The appropriate density \(N\) is achieved by adjusting \(n_0\) (3).

2.1 REPULSIVE SYSTEMS. — As a reference for the attractive case, we briefly recall well known results. For a strict repulsion, \(V(r) > 0\), a pure pair state is known to be impossible [5]. The ground state necessarily has a particle condensate, with \(n_0 \approx N\) if \(V_k\) is small. (For a moderately strong coupling, \(\Delta_k > 0\), while \(x_k < 0\).) Solutions (11) and (12) were obtained many years ago by Girardeau and Arnowitt [8], using the same variational approach. According to (11) and (17), we have

\[
\xi_0 = n_0 V_0 - \sum_k V_k x_k \quad \text{and} \quad \Delta_0 = n_0 V_0 + \sum_k V_k x_k
\]

from which a finite energy gap follows at once

\[
E_0 = \left[ 4n_0 V_0 \sum_k V_k |x_k| \right]^{1/2}. \tag{18b}
\]

That gap is known to be an artefact of the mean field approximation, implicit in (7) : it would disappear in more elaborate treatments [16]. Physically, the existence of a particle condensate couples the one particle states to the collective mode spectrum : elementary excitations pertain to the two modes simultaneously. The long wavelength Bogoliubov quasiparticles are nothing but density fluctuations. The latter are necessarily gapless (they are the Goldstone modes

(3) The totally condensed state \(n_0 = N\) is always unstable towards particle excitation in states with finite momentum. That follows from the linear term \(n_0 x_k\) in (7), which is dominant when \(\lambda_k\) is small. As a result, the solution of (16), if it exists, will always be such that \(n_0 < N\).
associated to the broken gauge symmetry). Hence $E_0 \equiv 0$ as soon as $n_0 \neq 0$. In contrast, when $n_0 = 0$ density fluctuation couple only to quasiparticle pairs: nothing prevents a gap in the one particle spectrum.

Putting aside the spurious result (18), the Girardeau Arnowitt mean field approach provides a sensible description of short wavelength properties.

2.2 Dilute Attractive Gases. — Let us assume that the attraction between two bosons is strong enough to produce a bound state (a feature which still permits a short range repulsive core). At low densities, we may expect that the bosons will first form « molecules », which will eventually Bose condense when the temperature goes to zero. Our variational ansatz (4) does describe such a situation, as shown in another context by Kjeldysh and Kozlov [10]. We set $n_0 = 0$ and we assume that $\lambda_k$ is small ($\sim N^{1/2}$). We may then expand (9):

$$x_k = \sqrt{n_k} + \frac{1}{2} n_k^{3/2} + \cdots.$$  

The ground state energy (7) thus takes the form

$$E_0 = \sum_k \epsilon_k n_k + \frac{1}{2} \sum_{k,k'} V_{kk'} \sqrt{n_k n_{k'}} +$$
$$+ \frac{1}{2} N^2 \nu_0 + \frac{1}{4} \sum_{k,k'} V_{kk'} \sqrt{n_k n_{k'}} \left[\sqrt{n_k} + \sqrt{n_{k'}}\right]^2 + \cdots$$

(19)

The first line in (19) is $\sim N$, the next one is $\sim N^2$, etc... It is convenient to put aside the Hartree term $1/2 N^2 \nu_0$ it being understood that it contributes a term $N \nu_0$ to the chemical potential: $\mu = \bar{\mu} + N \nu_0$.

Let us first consider terms of order $N$. We minimize $(E_0 - \mu N)$ with respect to $\sqrt{n_k}$. We thus obtain

$$2 \epsilon_k - 2 \bar{\mu} \sqrt{n_k} + \sum_{k} V_{kk'} \sqrt{n_{k'}} = 0.$$  

(20)

The homogeneous equation (20) is nothing but the Schrödinger equation for the internal wavefunction of a boson pair with total momentum zero. The corresponding eigenvector fixes $n_k$, within a normalization chosen so that $\sum n_k = N$; the eigenvalue fixes the chemical potential, which in that order does not depend on $N$. Let $\epsilon_{k0}, \psi_{k0}$ be the energy and wave function of the lowest bound state of two bosons. The solution of (20) is

$$\sqrt{n_k} = \sqrt{N} \psi_{k0}$$
$$\bar{\mu} = \frac{\epsilon_{k0}}{2} < 0$$

(21)

(the chemical potential of a pair is $2 \bar{\mu}$ : hence the factor $1/2$ in (21)). (21) describes a set of independent molecules, condensed in the state of zero total momentum. (Note that $\psi_{k0}$ is real and positive.)

We proceed to the next order in $N$. The minimization equation (20) is replaced by the non linear form:

$$2(\epsilon_k - \bar{\mu}) \sqrt{n_k} + \sum_{k,k'} V_{kk'} \sqrt{n_{k'}} = - 2 A_k$$
$$A_k = \sum_{k,k'} \frac{V_{kk'}}{4} \sqrt{n_k} \left[3 n_k + 4 \sqrt{n_k} n_{k'} + n_{k'}\right].$$

(22)

We look for a solution

$$\bar{\mu} = \frac{\epsilon_{k0}}{2} + \delta \bar{\mu}, \quad \sqrt{n_k} = \sqrt{N} \psi_{k0} + \nu_k$$

in which $\delta \bar{\mu}$ and $\nu_k$ are small corrections (respectively $\sim N$ and $N^{3/2}$). In lowest order, we do not need $\nu_k$: $\delta \bar{\mu}$ follows at once by projecting the first equation (22) onto $\psi_{k0}$:

$$\delta \bar{\mu} = \frac{1}{\sqrt{N}} \sum_k A_k \psi_{k0} = N \sum_{k,k'} \left[\psi_{k0}^2 \psi_{k0}^3 + \psi_{k0}^3 \psi_{k0}\right].$$

(23)

Restoring the Hartree term, we find a net change

$$\delta \mu = \delta \bar{\mu} + N \nu_0$$

$\epsilon_p = 4 \delta \mu N$ represents the interaction energy of two bound pairs, both with zero total momentum. Translating (23) into real space, we find

$$
\epsilon_p = \int dr_1 dr_2 ds_1 ds_2 \psi(r_1 - r_2) \psi(s_1 - s_2) \sum_{k,k'} V(r_1 - s_1) \times
$$
$$\times \left[\psi(r_1 - r_2) \psi(s_1 - s_2) + \psi(s_1 - r_2) \psi(r_1 - s_2) + \psi(r_1 - s_1) \psi(r_2 - s_2)\right]$$

$\epsilon_p$ is indeed the interaction energy, taking due account of symmetrization.

For a pure attraction, such that $V_k < 0$, $\delta \mu$ is obviously $< 0$: the ground state is unstable with respect to density fluctuations. If the interaction contains a repulsive core, the sign of $\delta \mu$ is not obvious. It seems that regions where $V < 0$ are favoured for purely geometrical reasons. Our guess is that an attraction strong enough to bind a boson pair cannot preserve a positive compressibility. The system will
collapse until the particles feel their repulsive core. Such a statement needs proof, however; we ignore the difficulty by working at constant $N$ \( (4) \).

The gap in the excitation spectrum is

\[
E_0 = \sqrt{\xi_0^2 - A_0^2} \approx \xi_0 - \frac{A_0^2}{2 \xi_0}
\]

where $\xi_0$ and $A_0$ are given by \( (11) \):

\[
\xi_0 = -\bar{\mu} + N \sum_k V_k \psi_{k0}^2
\]

\[
A_0 = \sqrt{N} \sum_k V_k \psi_{k0} = \sqrt{N} (-2 \xi_0) \psi_{00}.
\]  

In lowest order, $\bar{\mu} = \varepsilon_0/2$ : \( 2E_0 \) is just the energy $|\varepsilon_0|$ needed to break a single bound pair. In next order, there appears a small correction of order $N$:

\[
\delta E_0 = -\delta\bar{\mu} + N \sum_k V_k \psi_{k0} [\psi_{k0} + \psi_{00}].
\]  

The second term of \( (25) \) is usually $< 0$ : it may overcome the increase of $E_0$ due to the negative shift of $\bar{\mu}$. We could not produce a general proof of that feature --- but indeed in all the examples we considered, $\delta E_0$ was $< 0$ (see § 2.4). Despite the increase in $|\bar{\mu}|$, the energy gap goes down when the density $N$ increases. We conclude that the overlap of bound molecules opposes pair condensation: individual bosons exchange from one pair to another, and the molecules progressively lose their identity. At some critical density $N_c$, the gap $E_0$ should close to 0: we should then turn to a particle condensation regime ($\varepsilon_0 = 0$), as discussed before. The critical density will correspond to $\xi_0 A = 0$ : according to \( (24) \) that implies:

\[
N_c \psi_0^2 \sim 1.
\]  

Since the radius of a bound molecule is $\sim (\psi_0)^{-3/2}$, the critical density corresponds to close packing of these molecules. Pair condensation will disappear when the pairs overlap appreciably --- a plausible result indeed.

From that study of the dilute gas, we conclude that:

(i) Pure pair condensation only occurs if the attraction is strong enough to produce a bound state (otherwise, there is no natural unit of length that could define the spread of $n_k$).

(ii) Increasing $N$ seems to oppose pair condensation (a general proof that $\delta E_0 < 0$ would be desirable).

2.3 Attractive Systems Past the Zero Gap Threshold. --- Equation \( (18a) \) still holds, but now $x_k$ is $> 0$. As a result

\[
\xi_0 = \varepsilon_0 V_0 - \sum_k V_k \sqrt{n_k(n_k + 1)}
\]

\[
E_0 = -4 \varepsilon_0 V_0 \sum_k V_k \sqrt{n_k(n_k + 1)}.
\]  

If $\varepsilon_0$ and $V_k$ are both negative, the gap $E_0$ is pure imaginary: as expected, the density instability is reflected in the quasiparticle spectrum. Our mean field solution is then meaningless. (The fact that $E_0 \neq 0$ is also an artefact of the Girardeau Arnowitt type.)

In practice, we know that $\varepsilon_0$ cannot be $< 0$ (that would lead to the Hartree collapse mentioned earlier). Except for the spurious gap, the solution \( (27) \) is then physically sensible. The physical model is however completely unrealistic, and it does not deserve much discussion \( (5) \).

2.4 An Explicit Separable Interaction Model. --- In order to illustrate the disappearance of pair condensation, we consider the simple, separable interaction used in the BCS theory of superconductors

\[
V_{kk'} = \begin{cases} V & \text{if} \ e_k e_{k'} < D \\ 0 & \text{otherwise}. \end{cases}
\]  

We are aware that such an interaction is unrealistic. We use it for convenience as it displays the right qualitative behaviour with a minimum of complexity. The parameters are the strength $V$ and the cut off $D$. The dispersion equation for the bound state energy $\varepsilon_0$ is

\[
1 + V \sum_k \frac{1}{2 \varepsilon_k - \varepsilon_0} = 0.
\]  

(From now on, all $k$-summations are understood to run over the range $\varepsilon_k < D$.) For our parabolic band, the one boson density of states is $\nu(e) = a\sqrt{e}$ : \( (28) \) has a solution only if the attraction is strong enough:

\[
V < V^* = -\frac{1}{a\sqrt{D}}.
\]  

We assume that the condition \( (29) \) is met.

\( (4) \) Such a procedure does not create major difficulties as long as $n_0 = 0$. The density instability would show as collective modes with imaginary frequency, but collective modes do not appear in a mean field approximation anyway. This is no longer true when $n_0 \neq 0$ : then quasiparticles are directly hybridized with density fluctuations. A negative compressibility should lead to an imaginary $E_k$. As we shall see later, that does indeed happen.

\( (5) \) As a mathematical exercise, we may note that when $V_0 < 0$ the condensate fragments spontaneously in order to lower the energy. That affects the chemical potential, and therefore $\xi_0$ which becomes

\[
\xi_0 = A_0 = -\varepsilon_0 V_0 - \sum_k V_k x_k > 0.
\]  

The gap $E_0$ is identically 0, a point which has been noted by many authors. Since such a state is always unphysical, the point is irrelevant.
With such an interaction, the order parameter $A_k$ is $k$ independent (in the relevant range $\varepsilon_k < D$), as well as the difference $\gamma = \xi_k - \varepsilon_k$. We can choose the quantities $\gamma$ and $A$ as the two variational parameters that determine the ground state wave function. Let us define the auxiliary quantities

$$X(\gamma, A) = \sum_k n_k, \quad Y(\gamma, A) = \sum_k \sqrt{n_k(n_k + 1)}.$$  \hspace{1cm} (30)

For a pure pair condensate ($n_0 = 0$), $A$ must obey the self consistency equation

$$A = VY < 0.$$ \hspace{1cm} (31)

The other parameter is chosen so that $X = N$ (there is no need to introduce a chemical potential). We may rewrite (31) explicitly as

$$f = -\frac{Y}{A} = \frac{1}{2} \sum_k \frac{1}{\sqrt{(\varepsilon_k + \gamma)^2 - A^2}} = -\frac{1}{V}. \hspace{1cm} (32)$$

For a given $\gamma$, $f$ is an increasing function of $A$, sketched on figure 1. The lower limit $f_0$ corresponds to the dilute gas, the upper limit $f_m$ to the appearance of a particle condensate (closing of the gap). Explicit expressions are easily found for a parabolic band:

$$f_0 = \alpha \left[ \sqrt{D} - \sqrt{\gamma \text{ Arctg} \left( \sqrt{\frac{D}{\gamma}} \right)} \right],$$

$$f_m = \alpha \left[ \sqrt{D + 2 \gamma} - \sqrt{2 \gamma} \right]. \hspace{1cm} (33)$$

The range of $V$ for which a solution exists is shown on figure 2. There is no solution at all if $V > V^*$, irrespective of the density $N$. When $V < V^*$, $\gamma$ must lie in a finite range $(\gamma_1, \gamma_2)$. The lower bound $\gamma_1$ is the dilute limit ($-2 \gamma_1$ is the binding energy of a single pair with coupling $V$). The upper bound $\gamma_2$ fixes the threshold density $N_c$ at which $n_0$ appears. An equivalent representation of that solution is shown on figure 3, drawn in the « variational plane » spanned by $|A|$ and $\gamma$. $N_c(\gamma_2)$ is easily found by setting $\gamma = |A| = \gamma_2$ in (30). We may then eliminate $\gamma_2$ in order to obtain $N_c$ as a function of $V$. The result is shown on figure 4.

For large coupling strength, $N_c \sim x^2 D^2 V/8$. 

Fig. 1. — Graphical solution of (32).

Fig. 2. — The domain of existence of a pure pair condensate ground state (shaded area). The lower bound $V_1$ corresponds to $A = 0$ (dilute gas); the upper bound $V_2$ is the gapless limit $|A| = \gamma$. For large values of $\gamma$, $V_1 \sim -3 \gamma/aD^{3/2}$, while $V_2 \sim -\sqrt{8 \gamma/aD}$.

Fig. 3. — A graphical display of the solution in the space spanned by the two variational parameters $\gamma$, $|A|$. The shaded area is forbidden (it would produce an imaginary $E_0$). The dashed curves correspond to constant densities $N$. The full curve is the result of minimization for a given coupling strength $V$: the solution exists only in a finite range $(\gamma_1, \gamma_2)$.

Fig. 4. — The critical density for pair condensation as a function of coupling strength $V$. Close to $V^*$,

$$N_c \sim \frac{x^2}{6} \left[ (V - V^*) D \right]^2.$$
As long as $\gamma \leq D, N_e$ is of order $\alpha y^{3/2}$. If we remember that the spatial extent of a bound state with energy $\gamma$ is of order $r \sim \sqrt{h^2/\gamma}$, we see that $N_e \sim 1/r^3$ : as expected, the threshold is reached when bound boson pairs overlap.

The stability of that solution is discussed in Appendix A, using a slightly modified version of our variational argument. Expressed as a function of $N$ and $Y$, the ground state energy $E_0$ is a stable minimum with respect to $Y$ at constant $N$. On the other hand, $d^2E_0/dN^2$ is negative, leading as expected to unstable density fluctuations.

3. Spin 1 Bose liquids. — Let us consider bosons with an internal degree of freedom : they are characterized by a creation operator $a^*_{k\alpha}$ where $k$ is the momentum and $\alpha$ the internal state (at this stage, we do not specify the nature of the internal states : our discussion is general). Our variational ansatz (4) for the ground state wave function is generalized into :

$$|\psi_0\rangle = \frac{1}{N_c} \exp\left[ \phi_x a^*_{0\alpha} + \sum_k \lambda_{s\alpha}(k) a^*_{s\alpha} a_{-s\alpha} \right] |\text{vac}\rangle$$

(34)

The particle condensate (if any) is characterized by a vector $\phi_x$, while pairs $(k, -k)$ need a matrix $\lambda_{s\alpha}$ for their specification. Both $\phi_x$ and $\lambda_{s\alpha}$ may be complex.

An ordinary particle condensation regime is obtained if $\phi_x \neq 0$. We note that all condensed particles have the same internal state, a crucial feature of Bose condensation. Such a state necessarily breaks rotational symmetry : the condensate points toward some specific direction in $\alpha$ space. As usual, the particle condensate $\phi_x$ will «force» appearance of pair terms $\lambda_{s\alpha}(k)$ (Bogoliubov approximation). The matrix structure of $\lambda_{s\alpha}$ reflects the symmetry of $\phi_x$.

A pair state corresponds to $\phi_x = 0$. The complex matrix $\lambda_{s\alpha}$ must then be found self-consistently. Contrary to the previous case, $\lambda$ may be the unit matrix : a pair state may be invariant under rotations (pairs then form in a singlet state). That is not necessarily so, of course : anisotropic pair states exist as well (6).

Before putting any dynamics in the problem, we must normalize $|\psi_0\rangle$ and calculate relevant expectation values. This is straightforward for the single particle condensate, since the different states $\alpha$ factorize in $|\psi_0\rangle$. Our former result (6) becomes simply

$$\langle a_{0\alpha} \rangle = \phi_x \rightarrow \begin{cases} \langle n_{s\alpha} \rangle_{s\alpha} = \langle a^*_{0\alpha} a_{0\alpha} \rangle = \phi_{s\alpha}^* \phi_{s\alpha} \\ \langle x_{s\alpha} \rangle_{s\alpha} = \langle a_{0\alpha} a_{0\alpha} \rangle = \phi_{s\alpha} \phi_{s\alpha} \end{cases}$$

(35)

In order to normalize the pair terms $k \neq 0$, we limit ourselves to isotropic orbital states ($L = 0$), for which $\lambda_{s\alpha}(k)$ is an even function of $k$. Such states are likely to provide the maximum binding. From the definition (34), it then follows that $\lambda_{s\alpha}(k)$ is a symmetric matrix (possibly complex). Such matrices may be diagonalized by the transformation (7)

$$\hat{\lambda} = \bar{U} \hat{\lambda} U$$

where $U$ is an appropriate unitary matrix, $\bar{U}$ its transpose (note that $U$ may depend on $k$). Let us change the spin basis by defining

$$b^*_{s \alpha} = U_{s\alpha} a^*_{k\alpha}.$$

The wave function (34) becomes

$$|\psi_0\rangle = \frac{1}{N_c} \exp\left[ \phi_x a^*_{0\alpha} + \sum_k \lambda_{s\alpha} b^*_{s\alpha} b_{-s\alpha} \right] |\text{vac}\rangle$$

Performing the inverse transformation, we obtain the matrices $\bar{n}_k$ and $\bar{x}_k$ in the original basis

$$\bar{n}_{s\alpha} = \langle b^*_{s\alpha} b_{s\alpha} \rangle = \frac{1}{1 - |\lambda_{s\alpha}|^2}, \quad \bar{x}_{s\alpha} = \langle b_{s\alpha} b_{-s\alpha} \rangle = \frac{\lambda_{s\alpha}}{1 - |\lambda_{s\alpha}|^2}. \quad (36)$$

(6) Symmetry breaking Bose condensation is familiar in physics. The standard example is superfluid $^3$He, in which fermion pairs condense in a state $L = 1, S = 1$ [17]. Similar effects are expected in atomic hydrogen (stabilized by alignment of the electronic spin) : in the Bose condensed state, nuclear spins are polarized [18]. In much the same way, condensed excitons with an internal orbital or spin structure should display spectacular coherence effects [19].

(7) $\bar{U}$ is actually the transformation that diagonalizes the hermitian matrix $\hat{\lambda}^* \hat{\lambda} : \bar{U}^* \hat{\lambda} \bar{U}^* = D$. From the symmetry of $\hat{\lambda}$, it follows that $D = \bar{U}^* \hat{\lambda} \bar{U}^* \bar{U}$. We calculate the commutator $[\bar{D}, \hat{\lambda}] = [\bar{D}, \bar{U}^* \hat{\lambda} \bar{U}^* \bar{U}]$. Using one form of $\bar{D}$ in each term, we find it is zero : $\hat{\lambda}$ is therefore diagonal. Adjusting $\bar{U}$, one can make it real and positive : the basic ingredients of $\lambda_{s\alpha}$ are the positive numbers $\lambda_{s\alpha}$ (whose squares are the eigenvalues of $\hat{\lambda}^* \hat{\lambda}$).
The $\hat{\lambda}$ characterize the physical nature of the pairs. If only one $\hat{\lambda}$ is $\neq 0$ — say $\hat{\lambda}_1$ — we have a pure state: the two bosons have the same internal spin state, with a wave function $U_{1\lambda}$. The particle condensate described by (35) is of precisely that type: two of them make a pair in a pure state. When several $\hat{\lambda}$ are $\neq 0$, we have a mixture. The extreme case is $\hat{\lambda} = 1$: the spin structure then appears only in $x_k$ ($n_k$ is a unit matrix).

As in the preceding section, we may consider pseudocondensates, in which pairs accumulate either in the state $k = 0$, or in a small number of states ($\ll N$) close to $k = 0$ (it makes no difference to the energy). The occupancy matrices $n_{0\lambda}$ and $x_{0\lambda}$ may then be mixtures, in contrast to plain particle condensation which always corresponds to pure states (for instance, a pseudocondensate may be isotropic, while a real condensate cannot). Such an additional degree of freedom makes pseudocondensates more appealing: still, we shall see that they do not occur in the examples we consider.

Until now, our discussion was completely general. We now specialize to the case of spin 1 bosons. A rotation invariant pair interaction depends only on the operators $\hat{S}_1^x, \hat{S}_1^y, \hat{S}_1^z, (\hat{S}_2^x, \hat{S}_2^y, \hat{S}_2^z)$; the corresponding three coefficients fix the energy of the three spin states with total momentum $S = \hat{S}_1 + \hat{S}_2 = 0, 1, 2$. In practice, we are concerned only with orbitally even states (bonding), which because of statistics are consistent with $S = 0, 2$: there exists only two independent couplings. For convenience, we ignore the $(\hat{S}_1^x, \hat{S}_2^y)$ interaction, and we use the following basic hamiltonian:

$$H = \sum_k \frac{h^2 k^2}{2m} a_ka_k^\dagger + \frac{1}{2} \sum_{q} [V_q \rho_q - q + J_q S_q, S_{-q}]$$

$$\rho_q = \sum_k a_k^\dagger a_{k-q}, \quad S^i_q = \sum_k S^i_k a_k^\dagger a_{k-q}. \quad (38)$$

We now have two independent parameters, the scalar and exchange interactions, $V_q$ and $J_q$.

Spin 1 states are described in the cartesian basis, i.e. the three eigenstates such that $S_x, S_y, S_z$ are respectively zero. An arbitrary state is characterized by a complex vector, $\Psi_1, i\Psi_2$, normalized so that $|\Psi_1|^2 + |\Psi_2|^2 = 1$. The expectation value $\langle S \rangle$ is then $2\Psi_1 \cdot \Psi_2$. The angle between $\Psi_1$ and $\Psi_2$ fixes the state of polarization of the spin. $\Psi_1$ and $\Psi_2$ parallel yields linear polarization in the plane of $\Psi_1$ and $\Psi_2$

A boson pair is characterized by a $3 \times 3$ matrix $\lambda_{\alpha\beta}$. The isotropic $S = 0$ state is a perfect mixture corresponding to the unit matrix $\lambda = 1.0$. The corresponding interaction matrix element is $(V_q - 2 J_q)$. At the other extreme, the $S = 2$ states are pure states, made up with circularly polarized one particle states (consider for instance the $m = 2$ component in the usual $(l, m)$ representation: it is made up with two identical $m = 1$ circular states). The corresponding interaction is $(V_q + J_q)$.

The ground state energy in the mean field ansatz (34) involves the usual Hartree, Fock and Bogoliubov terms. In the absence of a particle condensate, it takes the form

$$E_0 = \xi_k \text{Tr} n_k + \frac{1}{2} V_0 \text{Tr} n_k \text{Tr} n_k + \frac{1}{2} J_0 \text{Tr} (n_k S^i \text{Tr} (n_k S^i))$$

$$+ \frac{1}{2} J_k \text{Tr} (n_k S^i \text{Tr} (n_k S^i))$$

$$+ \frac{1}{2} V_k \text{Tr} (n_k S^i \text{Tr} n_k S^i) + \frac{1}{2} J_k \text{Tr} (n_k S^i \text{Tr} n_k S^i)$$

$$+ \frac{1}{2} V_k \text{Tr} (n_k S^i \text{Tr} n_k S^i) + \frac{1}{2} J_k \text{Tr} (n_k S^i \text{Tr} n_k S^i)$$

(39) remains valid for a fully fragmented one particle condensate: we need only include $\delta$-function contributions $n_0$ and $x_0$ in the distributions $n_k$ and $x_k$. In the more usual case of non fragmented condensates, we should omit the Fock and Bogoliubov interactions inside the condensate (see section 2).

The actual ground state is obtained by minimizing (39). The resulting equations are similar to (12), except that $\xi_k$ and $\lambda_k$ are now spin operators

$$\frac{\delta E}{\delta n_k} = \xi_k = (\epsilon_k - \mu + NV_0) \frac{1}{2} + J_0 M^i \cdot S^i +$$

$$+ \sum_k \{ V_k \text{Tr} n_k + J_k \text{Tr} (n_k S^i \text{Tr} n_k S^i) \}$$

$$\frac{\delta E}{\delta x_k} = \lambda_k = \sum_k [V_k \text{Tr} x_k + J_k \text{Tr} (x_k S^i \text{Tr} x_k S^i)]$$

$$(M^i = \text{Tr} (S^i n_k)$ is the net ground state magnetization). $\xi_k$ and $\lambda_k$ define an effective $6 \times 6$ hamiltonian for momentum $k$, whose ground state fixes $\xi_k$. In practice, the following identity holds for an arbitrary operator $A$ when expressed in the cartesian basis:

$$\sum_k \xi^i_k A S^i = (\text{Tr} A) - \xi_k$$

(41) (one proves (41) by using the representation $(S^i)^{\alpha\beta} = i\delta^{\alpha\beta}$). As a result, a simple solution corresponds to $\xi_k, \lambda_k, n_k, x_k$ simultaneously diagonal (the matrix $U$ in (37) is then unity). If there is a net magnetization $\lambda$, say along the z-axis, all these operators must also commute with $S_z$ in order to avoid Larmor precession around the exchange field. More generally, we only consider the simple case in which $U$ is $k$-independent: that includes singlet pairs ($\xi_k = 1$), pure pair states with either linear ($S_z = 0$) or circular ($S_z = 1$) polarization. We also assume $V_q > 0, V_q - 2 J < 0$.

3.1 Pure pair condensation in the singlet state.

We first consider the case $\phi_k = 0$. We moreover assume that boson pairing occurs in the $S = 0$ state: $n_k$ and $x_k$ are unit matrices, represented by $c$-num-
bers \(n_k\) and \(x_k\). The energy (39) simplifies considerably. Noting that \(S' = - S'\), we find

\[
E_0 = 3 \sum_k \epsilon_k n_k + \frac{V_0 N^2}{2} + 3 \left[ V_{k-k'} [n_k n_{k'} + x_k^* x_k] + J_{k-k'} [n_k n_{k'} - x_k^* x_k] \right] \tag{42}
\]

(in which \(N = 3 \sum n_k\)). The problem is similar to section 2, except for the different couplings \((V \pm 2 J)\) in the Fock and Bogoliubov terms.

The solution has again the form (12), \(\xi_k\) and \(A_k\) involving respectively \((Y \pm 2 J)\) instead of \(Y\) (as in section 2, we choose \(x_k\) real and positive). The solution makes sense only if the quasiparticle energy \(E_k\) is real, i.e. if \(\xi_0 > |A_0|\), a condition which implies

\[
\sum_k \left[ V_k [n_k + x_k] + 2 J_k [n_k - x_k] \right] + NV_0 - \mu > 0
\]

(43)

(compare with our former result (14)).

In order to study the stability of that solution with respect to single particle condensation, we add to \(n_k, x_k\) a small condensate correction \(n_0, x_0\). In first order, it does not matter whether that condensate is fragmented or not: the matrix structure of \(n_0\) is arbitrary. We write it in the general form (37), noting that macroscopic occupancy implies \(\tilde{x} \approx 1\), i.e. \(\tilde{n} = \tilde{x}\). Thus

\[
n_0 = U_0^* \tilde{n}_0 U_0, \quad x_0 = U_0^* \tilde{n}_0 U_0. \tag{44}
\]

Since \(F_0 = E_0 - \mu N\) is already minimized with respect to \(n_k\), the first order correction arises only from the explicit dependence upon \(n_0\) (the accompanying change in \(n_k\) would enter in second order). The resulting change in \(F_0\) is therefore

\[
\Delta F_0 = (NV_0 - \mu) \text{Tr} \tilde{n}_0 + \sum_k V_k [n_k \text{Tr} \tilde{n}_0 + x_k \text{Re Tr} \tilde{x}_0] + \sum_k J_k [n_k \text{Tr} \tilde{S}_k^2 \tilde{n}_0 \tilde{S}_0^2 + x_k \text{Re Tr} \tilde{S}_k^2 \tilde{x}_0 \tilde{S}_0^2].
\]

Making use of (44), we transform that expression into

\[
\Delta F_0 = \left[ NV_0 - \mu + \sum_k (V_k + 2 J_k) n_k \right] \text{Tr} \tilde{n}_0 + \sum_k (V_k - 2 J_k) x_k \text{Re Tr} (\tilde{n}_0 W) \tag{45}
\]

where \(W = U_0^* U_0\) is a symmetric unitary matrix. In the present « bonding » case, \((V - 2 J) < 0\), (45) is lowest when we choose \(W = 1\) (remember that \(n_0\) is positive definite). The stability requirement that \(\Delta F_0 > 0\) is then identical with (43). As in section 2, the existence of a finite gap \(E_0\) guarantees stability towards formation of a particle condensate (irrespective of its shape). Closing of the gap will mark the birth of such a condensate.

3.2 THE LOW DENSITY LIMIT. — The distribution \(n_k\) is then \(\ll 1\). We could expand (42) directly in powers of \(x_k \approx \sqrt{n_k}\). Actually, it is simpler to carry over the results of section 2.2. The only difference is the replacement of \(V\) by \((V + 2 J)\) in the Fock term, by \((V - 2 J)\) in the Bogoliubov term. In lowest order, the extremum equation (20) becomes

\[
2[x_k - \mu] \sqrt{n_k} + \sum_k (V - 2 J)_{kk'} \sqrt{n_k} = 0 \tag{46}
\]

(46) is the Schrödinger equation that describes a bound boson pair in the singlet state \(S = 0\). Let \(\epsilon_0 < 0\) and \(\Psi_{k0} > 0\) be the energy and internal wave function of that bound state. The solution of (46) is

\[
\mu = \frac{\epsilon_0}{2}, \quad \sqrt{n_k} = \frac{3}{N} \Psi_{k0}^*.
\]

In next order, we must first add to \(\mu\) the Hartree term \(NV_0\). Moreover, (46) acquires inhomogeneous terms, as in (22); the left hand side is now equal to \(-2A_k\), where

\[
A_k = \sum_{k'} \left\{ (V + 2 J)_{kk'} \sqrt{n_k n_{k'}} + (V - 2 J)_{kk'} \times \sqrt{n_k} \frac{3}{4} n_k + \frac{n_{k'}}{4} \right\}. \tag{48}
\]

The resulting shift of \(\mu\) is obtained by projecting (46) on the ground state \(\Psi_{k0}\). Altogether, we find

\[
\mu = \frac{\epsilon_0}{2} + NV_0 + \delta \mu
\]

\[
\delta \mu = \sum_{kk'} \Psi^*_{k0} [V_{kk'}(\Psi_{k0} + \Psi_{k'0})^2 - 2 J_{kk'}(\Psi_{k0} - \Psi_{k'0})^2]. \tag{49}
\]

Making use of (44), we transform that expression into

\[
\Delta F_0 = \left[ NV_0 - \mu + \sum_k (V_k + 2 J_k) n_k \right] \text{Tr} \tilde{n}_0 + \sum_k (V_k - 2 J_k) x_k \text{Re Tr} (\tilde{n}_0 W)
\]

(49) (compare with (23)). We note that the spin coupling is much less efficient than the scalar one \((\delta)\): its contribution is reduced by a factor \((4/\mu)^2\), as compared to \((\mu + \psi)^2\). As a result, \(\delta \mu\) may well be positive,

\[
(\delta) \text{ An extreme case is that of a very long range interaction } J(r_1 - r_2), \text{ such that } J_{kk'} \text{ is localized near } k = k' = 0, \text{ in a region where } \Psi_k \text{ is constant. Then the spin term disappears completely in (49). That can be seen directly: the magnetic exchange interaction of two overlapping boson pairs, } (1, 2) \text{ and } (3, 4), \text{ is then position independent; it is simply } J(S_1 + S_2)(S_3 + S_4), \text{ identically zero since both pairs are singlets.}
even though \( V - 2J < 0 \). The existence of a bound state does not necessarily imply a negative compressibility. Anyhow, the Hartree term \( NV_0 \) is \( > 0 \), and it will usually dominate. We have thus achieved a physically sensible model of pair condensation. A single pair can bind into a singlet molecule — but then a third boson will only sense the average scalar repulsion: forces are automatically saturated.

As in section 2.2, we can calculate the gap

\[
E_0 \approx \xi_0 - \frac{A_0^2}{2N},
\]

Using (41) and (49), we find

\[
E_0 = |\epsilon_0| - \delta \mu + \frac{N}{3} \sum_k [(V_k + 2J_k) \psi_{k0}^2 + (V_k - 2J_k) \psi_{k0} \psi_{00}].
\]

(50)

Since the various terms of (50) have different signs, we cannot draw any firm conclusion. For short range interactions, the last term of (50) will usually dominate (the \( k \)-summation does not converge if \( V - 2J \) is constant). Then \( dE_0/dN < 0 \) : the gap decreases to 0 at some critical density \( N_c \).

### 3.3 Separable Interaction Model

As in section 2.4, we assume constant matrix elements \( V \) and \( J \) below a common cut off \( D \). Using the same definition (30) for \( X \) and \( Y \), we may write the energy (42) of our singlet pair state as

\[
E_0 = 3T + \frac{VN^2}{2} + \frac{3}{2}(V + 2J)X^2 + \frac{3}{2}(V - 2J)Y^2
\]

(51)

(compare with (A.4)). \( X = N/3 \) is fixed by the density : \( Y \) is the only variational parameter. Let us define

\[
\begin{align*}
V_1 &= 4V + 2J > 0 \\
V_2 &= V - 2J < 0
\end{align*}
\]

(52)

The ground state energy is given by

\[
E_0 = T + \frac{V_1X^2}{2} + \frac{V_2Y^2}{2}
\]

(53)

It differs from (A.4) only because \( V_1 \neq V_2 \).

At constant \( N \), only \( V_2 \) is relevant. The discussion of section 2.4 is unchanged : the pair state exists if \( V_2 \) is strong enough to bind a molecule. Increasing the density opposes pair formation. At a critical density \( N_c \) (function of \( V_2 \) only), bound pairs dissociate and a one particle condensate appears (while the gap \( E_0 \) closes to zero). What is new is the calculation of the compressibility, i.e. of \( d\mu/dN \) which depends on both \( V_1 \) and \( V_2 \). We show in appendix A that \( d\mu/dN \) is positive if \( V_1 \) is repulsive enough. The threshold \( V_1 = V_c > 0 \) can be calculated explicitly (see (A.11)). We reach again the same conclusion : binding and pair condensation are consistent with a positive compressibility.

Such a singlet pair state is stable with respect to small changes in \( Y \) (see Appendix) or in \( X \) (density fluctuations). We should also check whether the singlet is indeed the best choice. If we allow for more complicated spin structures, \( X \) and \( Y \) become matrices : the energy must also be minimal with respect to distortion of these matrices. The ground state energy (39) now reduces to

\[
E_0 = \text{Tr} (T) + \frac{V}{2} [ (\text{Tr} X^2 + \text{Tr} X^2 + \text{Tr} Y^+ Y^+) + \frac{J}{2} \{ [\text{Tr} (X^2)]^2 + \text{Tr} (X^2 X^2) \\
+ \text{Tr} (Y^+ Y^+ Y^+ Y^+) \}
\]

(54)

We simplify it considerably by using the identity (41), together with

\[
\sum_i S_i^i \text{Tr} (AS_i^i) = A - \bar{A}
\]

(but are valid only in the cartesian basis). (54) then becomes

\[
E_0 = \text{Tr} \bar{T} + \frac{V + J}{2} [ (\text{Tr} X^2 + \text{Tr} X^2 + \text{Tr} Y^+ Y^+) - \frac{J}{2} [2 \text{Tr} (X\bar{X}) + \text{Tr} Y \bar{Y}] + (\bar{X} \text{ and } \bar{Y} \text{ are real and positive}). E_0 \text{ thus takes the final form}
\]

\[
E_0 = \text{Tr} \bar{T} + \frac{V + J}{2} [ (\text{Tr} X^2 + \text{Tr} X^2 + \text{Tr} (\bar{X}^2 + \bar{Y}^2)] - \frac{J}{2} [ \text{Tr} \bar{W} \bar{W} + 2 \text{Tr} (\bar{X} \bar{W} \bar{X} \bar{W}^+)]
\]

(58)

where \( W = U\bar{U} \) is unitary and symmetric. (Each component \( T_\alpha \) is related to \( \bar{X}_\alpha \) and \( \bar{Y}_\alpha \) by the relationship (A.2) established for a single channel).

We first remark that \( \bar{W} \) only enters the last term of (58). Since \( J > 0 \), the energy will be minimal if we choose \( \bar{W} = \frac{1}{2} \) (remember that \( \bar{X}_\alpha \) and \( \bar{Y}_\alpha \) are all
The solution is still determined within an arbitrary orthogonal matrix \( U \) (such that \( U = U^* \)) : that freedom corresponds to a genuine degeneracy, arising from rotation invariance. In what follows, we choose \( U = 1 \).

In the vicinity of the singlet state, we can decompose fluctuations \( \delta X \) and \( \delta Y \) into two decoupled parts:

- Scalar corrections \( \delta X \) and \( \delta Y \). We already showed that the singlet was stable in that respect.
- Corrections such that \( \text{Tr} \delta X = \text{Tr} \delta Y = 0 \).

In the latter case, the relevant part of (58) reduces to

\[
E_0 = \text{Tr} \left[ \frac{1}{2} \left( V - J + V + J \right) \delta X^2 \right].
\]

The singlet ground state will be stable if for each component \( \alpha \) the second order corrections are positive definite:

\[
\frac{\text{Tr} \delta^2 X_\alpha}{2} + \frac{\text{Tr} \delta^2 Y_\alpha}{2} > 0. \tag{59}
\]

That condition may be analysed using the machinery of Appendix A. Stability is guaranteed if

\[
A = 1 + V(a + c) + J(c - a) + \delta(V^2 - J^2) > 0 \tag{60}
\]

(see appendix for notations). The condition (60) is certainly obeyed if \( V > J \). Actually, a tedious calculation shows that \( A > 1 \) whenever the compressibility is positive : in physically relevant situations, singlet pairing is the stable ground state.

### 3.4 Particle Condensation Past the Dissociation Threshold

\( \chi \) and \( \gamma \) now include a condensate part, \( \chi_0 \), \( \gamma_0 \), as well as the former pair contribution \( \chi_p \), \( \gamma_p \). Both have the general form (57) — *a priori*, the unitary transformations \( U_0 \) and \( U_p \) may be different. We may again write the energy \( E_0 \) in the form (58) : depending on the term considered, the matrix \( W \) will be one of the four combinations \( U_0 U_0 \), \( U_0 U_p \), \( U_p U_0 \), \( U_p U_p \). Since \( J > 0 \) is very clear that the energy will be minimal if all these \( W \) are equal to \( 1 \) \( \tag{10} \).

We recover the situation of the preceding section : in the ground state, the four matrices \( \chi_0 \), \( \chi_p \), \( \gamma_0 \), \( \gamma_p \) can be made diagonal, real and positive (in the cartesian basis), within an arbitrary orthogonal transformation which corresponds to a rotation of the axes. Such a spin configuration ranges from a pure linearly polarized state \( (\chi, \gamma) \) have only one element \( \neq 0 \), to a complete singlet mixture \( (\chi, \gamma) \) are unit matrices). Note that circularly polarized states are excluded from the outset : they cost too much exchange energy.

We shall only consider the two limiting cases, corresponding to the following matrix structures:

- Pure \( z \)-polarized state
- Singlet mixture

(\( I_z \) is the projector on the \( z \) state, \( I \perp = 1 - I_z \)). We consider first the pure state, which may or may not be fragmented. Actually, fragmentation does not affect the solution \( \chi_p \), \( \gamma_p \) : it only adds to \( E_0 \) the Fock and Bogoliubov intracondensate interactions. Returning to (54), one verifies easily that all the \( k = 0 \) terms are equal in such a pure state:

\[
E_f = E_{\text{Fock}} = E_{\text{Bog}} = \frac{V n_0^2}{2}. \tag{61}
\]

Since \( V > 0 \), fragmentation of a pure state will always cost energy. The only dilemma is between

- (i) a pure, non fragmented, \( z \)-polarized one particle condensate;
- (ii) a singlet fragmented mixture.

To answer that question, we consider the pure state energy, obtained from (58):

\[
E_0 = T + 2 \overline{T} + V \left[ \frac{N^2}{2} + n_0 (X_p + Y_p) + \frac{X_p^2 + Y_p^2}{2} + X_p^2 + Y_p^2 \right]
\]

\[
+ J [2 n_0 (\overline{X}_p - \overline{Y}_p) + 2 \overline{X}_p X_p + \overline{X}_p^2 - 2 \overline{Y}_p Y_p - \overline{Y}_p^2] \tag{62}
\]

\( N = n_0 + X_p + 2 \overline{X}_p \) is the total density, \( T \) and \( \overline{T} \) are the kinetic energies corresponding to \( X_p \) and \( \overline{X}_p \).

\( (\text{\textcopyright} \) Since \( |W_{\alpha\beta}| < 1 \), we have \( |\text{Tr} \delta W| < \text{Tr} \delta W \). The quantity \( (XW \delta W^+ ) \) may be written as:

\[
\sum_{\alpha \beta} |W_{\alpha\beta}|^2 \delta X_\alpha \delta X_\beta = \sum_{\alpha} \delta^2 X_\alpha - \frac{1}{2} \sum_{\alpha \beta} |W_{\alpha\beta}|^2 (X_\alpha - \overline{X}_\alpha)^2 < \text{Tr} \delta^2 X. \tag{59}
\]

\( (\text{\textcopyright} \) Such a conclusion is consistent with our former result (45) : the actual ground state corresponds to that condensate which turned unstable at the dissociation threshold, i.e. to \( U_0 U_0 = 1 \).
involves only \( \text{Tr } n_0 \) (see (45)) : it is the same in \( E_0^2 \) and in the singlet energy \( E_0^2 \). The only difference between these two energies arises from the \textit{intra} condensate interaction; according to (61)

\[
E_0 - E_0^2 = V n_0^2 > 0 .
\]

We conclude that the \textit{linearly polarized, non fragmented condensate} is the stabllest configuration.

From then on, the problem is mostly algebraic. We first express that (62) is stationary with respect to \( X_p, \overline{X}_p, Y_p, \overline{Y}_p \) at constant \( N \) (any change in \( X_p, \overline{X}_p \) must be balanced by a change in \( n_0 \)). Writing \( dT \) and \( d\overline{T} \) as in (A. 2), we obtain the following conditions

\[
\begin{align*}
\gamma &= V(n_0 - Y_p) + 2 J Y_p \\
\overline{\gamma} &= V(\overline{X}_p - X_p - Y_p) + J(X_p - \overline{X}_p + n_0 + 2 \overline{Y}_p) \\
\Delta &= V(n_0 + Y_p) - 2 J Y_p \\
\overline{\Delta} &= V \overline{Y}_p - J[n_0 + Y_p + \overline{Y}_p].
\end{align*}
\]

We may then expand near the dissociation threshold \( X_c, Y_c \), setting

\[
X_p = X_c + x, \quad \overline{X}_p = \overline{X}_c + \overline{x}
\]

(with similar definitions for \( y \) and \( \overline{y} \)). The set of equations (63) then appears as a \textit{linear} system in \( x, \overline{x}, y, \overline{y}, n_0 \), which may be examined in the language of Appendix A. The discussion is fairly tedious, and often we cannot draw firm conclusions without resorting to specific models; we shall only list a few relevant questions and the various answers that can emerge.

3.4.1 \textit{Energy gaps.} — The quasiparticle energies for the \( z \) and \((x, y)\) channels are respectively

\[
E_k = \sqrt{(\epsilon_k + \gamma)^2 - \Delta^2}, \quad \overline{E}_k = \sqrt{(\epsilon_k + \overline{\gamma})^2 - \overline{\Delta}^2}.
\]

Their \( k = 0 \) limit provides the gaps \( E_0 \) and \( \overline{E}_0 \) for elementary excitations. Our calculation makes sense only if \( E_0 \) and \( \overline{E}_0 \) are real, a condition which implies \( \gamma > |\Delta|, \overline{\gamma} > |\overline{\Delta}| \). From (63), we see that

\[
\begin{align*}
G &= \gamma - |\Delta| = 2 V n_0 \\
\overline{G} &= \overline{\gamma} - |\overline{\Delta}| = (V - J)(\overline{x} - x) + (V + J)(\overline{y} - y).
\end{align*}
\]

\( G \) is obviously \( > 0 \). It can be shown that \( \overline{G} \) is also positive whenever the previous stability conditions are met (\( \overline{G} > 0 \) indeed follows from the condition (60), \( \overline{A} > 1 \), which guaranteed stability of the singlet structure). In fact, that issue is partly semantic, since the gaps are artefacts of our mean field approximation. In the presence of a genuine \textit{one particle condensate}, quasiparticles coincide with the Goldstone modes arising from the ground state degeneracies. The two types of quasiparticles correspond respectively to \textit{gauge} and \textit{polarization} fluctuations : they should be gapless, such that \( E_0 = \overline{E}_0 = 0 \). We recover the same contradictions as in the Girardeau Amowitt description of repulsive systems. This point will be discussed in more detail elsewhere [14].

3.4.2 \textit{Density.} — For a given value of \( n_0 \), we can calculate \( x, \overline{x} \), and the corresponding correction to the density (compared to threshold)

\[
n = N - N_c = n_0 + x + 2 \overline{x} = x n_0 .
\]

The expression of \( \alpha \) is complicated : we shall not give it explicitly. \( \alpha \) may well be \( < 1 \) (meaning that the condensate « empties » the finite momentum states), or even \( \alpha < 0 \) : then there would exist \textit{two} solutions for a given \( N < N_c \), respectively with and without a one particle condensate \( n_0 \). The transition is then \textit{first order} (see next paragraph).

3.4.3 \textit{Chemical potential and compressibility.} — Past threshold, the chemical potential is simply

\[
\mu = \frac{\partial E_0}{\partial n_0} = V(X_p - Y_p) + J(\overline{X}_p - \overline{Y}_p) .
\]

One verifies easily that \( \mu \) is continuous at threshold, as expected. Near threshold, we can again carry a first order expansion

\[
\delta \mu = \mu - \mu_c = \beta n
\]

\( \beta \) is directly related to the compressibility. Once again, the explicit expression of \( \beta \) is messy, and we do not give it, since we cannot draw any firm conclusion.

![Fig. 5.](image-url)

(a)  (b)  (c)

The various possible behaviours, as a function of \( \alpha \) and \( \beta \), are shown on figure 5 (past threshold, the curves are parametrized by \( n_0 \)).

— Case (a) corresponds to \( \alpha > 0, \beta > 0 \). In such a case, one may show that \( \beta < 1 \) : appearance of a
particle condensate $n_0$ lowers the compressibility (such a result is consistent with the idea that the condensate lowers the energy). The transition from pair to particle condensation is then a smooth second order process.

— Case (b) corresponds to $\alpha > 0$, $\beta < 0$. Before reaching the threshold $N_c$, the pair state will undergo a first order transition, towards a particle state with a higher density. In drawing figure 5b, we assumed that $\mu(N)$ bends up again as $N$ increases (ultimately, the scalar repulsion should dominate). The plateau AB is then obtained by the usual Maxwell construction.

— The more exotic case (c) corresponds to $\alpha < 0$ (one can then show that $\beta > 1$). As stated before, there exist several solutions for a given $N$. If the curve $\mu(N)$ bends up for large $N$, we again expect a first order transition, with the usual Maxwell plateau AB (the fact that $\mu$ has a cusp at $N = N_c$ does not affect the thermodynamical argument).

At this stage, we could not decide between these possibilities. It seems that increasing $V$ favours case (c) — it may well happen that case (a) is always excluded. The question remains completely open. Probably, it can only be answered in specific models.

4. Conclusion. — The purpose of this paper was twofold. First, we draw attention to a simple saturation mechanism for attractive Bose liquids: rather than combining a short range repulsion with a long range attraction, it is much simpler to consider bosons with an internal degree of freedom. A local interaction may be attractive in a given spin state, while it remains repulsive on the average, thereby ensuring a positive compressibility.

Our second aim was to clarify the competition between particle and pair condensation. We have shown that pair condensation occurs only when the pair interaction is attractive enough to bind a pair of bosons into a molecule. At low density, the ground state is a Bose condensate of these molecules. As the density increases, overlap of two molecules opposes pair formation. At a critical density $N_c$, the gap for pair ionization vanishes: that threshold marks the onset of a one particle condensate $n_0$.

We studied in detail the case of spin 1 bosons coupled via an exchange interaction. In the pair regime, the ground state is isotropic (singlet pairs). Past threshold, the one-particle condensate breaks rotational symmetry: we show that the ground state corresponds to linearly polarized bosons. The condensate is a real one, with an order parameter $\langle \psi \rangle$: there is no fragmentation into a sharp peak of pair states near $k = 0$.

The properties of condensates that break rotation symmetry will be discussed elsewhere [14], both for particles with spin 1 and with double spin 1/2. That raises a number of interesting questions: nature of symmetry breaking, elementary excitations, etc...

Appendix A. — In the separable interaction model of section 2.4, the variational calculation may be cast in a more convenient form. We start from the definition (30) and we calculate the derivatives

$$
\frac{\partial X}{\partial A} = \frac{\partial Y}{\partial \gamma} = \sum_k \frac{A(e_k + \gamma)}{2 E_k^3} = b
$$

$$
\frac{\partial X}{\partial A} = -\sum_k \frac{A^2}{2 E_k^3} = -a, \quad \frac{\partial Y}{\partial A} = -\sum_k \frac{(e_k + \gamma)^2}{2 E_k^3} = -c.
$$

(A.1)

We note that $0 < a < b < c$. Moreover, the Jacobian

$$
\delta = ac - b^2 = \sum_k \frac{A^2 (e_k - e_\gamma)^2}{8 E_k^3 E_\gamma^3}
$$

is also positive. We also introduce the kinetic energy

$$
T = \sum_k \epsilon_k n_k.
$$

Calculating the derivatives $\partial T/\partial \gamma$ and $\partial T/\partial A$, we easily verify that

$$
dT = -\gamma dX - A dY
$$

(A.2)

suggests to take $X$ and $Y$ as our variational parameters, instead of $\gamma$ and $A$: then we simply have

$$
\frac{\partial T}{\partial X} = -\gamma, \quad \frac{\partial T}{\partial Y} = -A.
$$

(A.3)

For a pure pair state, $X = N$ is fixed: the only adjustable parameter is $Y$. The total energy, including the Hartree term, may be written as

$$
E_0 = T + VX^2 + \frac{1}{2} VY^2.
$$

(A.4)

It is extremal if

$$
\frac{\partial E_0}{\partial Y} = -A + Y = 0.
$$

We recover the condition (31) — which, by the way, may be cast in the form

$$
-\frac{1}{V} = \sum_k \frac{1}{2 E_k} = (c - a).
$$

(A.5)

The stability at constant $N$ is controlled by

$$
\frac{\partial^2 E_0}{\partial Y^2} = V - \frac{\partial A}{\partial Y} = V + \frac{a}{\delta}.
$$

(A.6)

Using (A.5), we verify that (A.6) is $\sim (b^2 - a^2) (c - a)$, which is always $> 0$. Our solution is indeed a minimum of $E_0$.

The compressibility is proportional to $d^2 E_0/dN^2$. In deriving (A.4), we must watch that the equilibrium value of $Y$ depends on $N$ via the cross terms in $T$. 

Appendix A.
The total derivative is therefore
\[
\frac{d^2E}{dN^2} = \frac{\partial^2 E}{\partial X^2} - \frac{(\partial^2 E/\partial X \partial Y)^2}{\partial^2 E/\partial Y^2} = \frac{2V - \frac{\partial^2}{\partial X} - \frac{(\partial^2 E/\partial Y)^2}{\partial^2 E/\partial Y^2} = 0}{(c - a)(b^2 - a^2)}.
\]

The coefficients in (A.7) are obtained by inverting the Jacobian matrix (A.1). Eliminating \(V\) with the help of (A.5), one verifies easily that
\[
\frac{d^2E}{dN^2} = \frac{3a^2 - 2b^2 - ac}{(c - a)(b^2 - a^2)} < 0.
\]

As expected, the attraction makes the system unstable.

We now consider spin 1 bosons condensing in a pure singlet pair state. Instead of (A.4), the energy is given by (53)
\[
E_0 = \frac{T + V_1X^2}{2} + \frac{V_2Y^2}{2}
\]

where \(V_1\) and \(V_2\) are independent couplings (the net density is \(N = 3X\)). The condensation process is controlled by \(V_2\) only; for instance, (A.5) is replaced by
\[
-\frac{1}{V_2} = (c - a).
\]

On the other hand, the compressibility involves both \(V_1\) and \(V_2\). Using (A.7) and (A.1), we find
\[
\frac{3d^2E}{dN^2} = V_1 + \frac{c}{\delta} \frac{b^2}{\delta(V_2\delta + a)}.
\]

We may use (A.9) in order to eliminate \(V_2\); we then find
\[
\frac{3d^2E}{dN^2} = \frac{V_1 + \frac{a}{a^2 - b^2}}{2}.
\]

If \(V_1\) is repulsive enough, such that
\[
V_1 > \frac{a}{b^2 - a^2} > 0
\]

the ground state will be stable, contrary to the spinless case.

References


[7] This point is discussed in detail by Comte, C., Nozières, P., J. Physique.
[16] The literature on that subject is very large. A consistent gapless solution was first obtained by Beliaev [2]. Mathematically, the condition \(E_0 = 0\) follows from a general theorem due to Hugenholtz, N. M., Pines, D., Phys. Rev. 116 (1959) 489. It can be verified to all orders in perturbation theory, Gavoret, J., Nozières, P., Ann. Phys. (N. Y.) 28 (1964) 349.

See also recent developments by Nepomnyashchy, Y. A., Nepomnyashchy, A. A., Sov. Phys. JETP 48 (1978) 493. The way in which spurious gaps appear in approximate theories is beautifully explained in the basic paper of Hohenberg and Martin [3].