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Exciton Bose condensation : the ground state of an electron-hole gas

I. Mean field description of a simplified model

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Résumé. — Nous considérons un gaz d'électrons et de trous dans un modèle simple de semi-conducteur, avec un gap direct et des bandes isotropes et non dégénérées. Nous étudions la condensation de Bose de ce système en fonction de la densité, négligeant dans une première étape l'effet d'écran et la structure de spin des porteurs. Nous décrivons ainsi le passage continu depuis le condensat de Bose d'excitons atomiques à basse densité jusqu'à l'état « d'isolant excitonique » — et finalement au plasma d'électrons et de trous libres à haute densité. Comparée aux théories existantes, notre formulation prend en compte l'appariement des électrons et des trous dans l'état fondamental, dans un langage simple et proche de la réalité.

Abstract. — We consider an electron-hole gas in a simple model semiconductor, with direct gap and isotropic, non degenerate bands. We study the Bose condensed ground state of that system as a function of density, using a mean field variational ansatz. In a first stage, we ignore screening as well as the spin structure of the carriers. We thus describe the smooth transition between Bose condensation of atomic excitons at low densities, and the « excitonic insulator » state and ultimately electron-hole plasma at high densities. As compared to previous treatments, our approach includes the effect of electron-hole pairing on the ground state, within a simple realistic ansatz.

1. Introduction. — Consider a semiconductor containing an equal number of conduction electrons and valence holes, N per unit volume. Such carriers may be produced by an appropriate pumping technique, or they may result spontaneously from an overlap of conduction and valence bands (monitored for instance by pressure). In the former case, one controls N , in the latter the chemical potentials; the physics remains basically the same. We assume that the carriers are cold ⁽¹⁾. We may then ask what is their ground state? How does it evolve with density? Does one expect density instabilities leading to a liquid-gas phase separation? These questions have received considerable attention in the past, the main landmarks being the work on Bose condensation

led by Kjeldysh [1-3] and by Kohn [4] in the late sixties (the so-called « excitonic insulator »), and the many papers on electron-hole droplet condensation in the seventies [5]. In the present paper, we take the issue again. Using a simplified model, we propose a variational ansatz which interpolates between low and high densities. We thus emphasize the smooth transition between Bose condensation of atomic excitons at one end, excitonic insulators and ultimately the normal electron-hole plasma in the other end. At that stage, we do not attempt to describe realistic materials: we rather wish to understand the many body aspects of an interacting electron-hole gas, taking into account the *tendency to form bound pairs* (a trend which is ignored in usual Hartree-Fock or RPA approximations). Similar interpolations have been carried out before [6] using essentially the same mean field approximation. Our language is somewhat simpler, and we feel that our variational ansatz is more realistic. Our approach is quite general, and it can be transposed to other problems. Instead of electron-hole pairing, one can study particle pairing in an attractive Fermi gas: one thereby describes the smooth transition between a weak coupling BCS superconductor on the one hand, and the Bose condensation of strongly bound « molecules » on

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⁽¹⁾ Such a statement may be quite unrealistic in pumped systems. Unless they are produced exactly at threshold, the carriers have a temperature which may be much higher than that of the lattice. They can be cooled only if their lifetime is longer than the energy relaxation time. Such a requirement is hard to meet, especially in direct gap materials in which the lifetime is short.

the other hand. In the same way, one can analyse the competition between particle and pair condensation in a Bose liquid [7]. These problems will be dealt with in separate papers.

Consider first a single electron-hole pair : it forms a bound pair, the *exciton*, whose energy $-\varepsilon_0$ and radius a_0 provide the natural units of the problem. Two excitons may in turn bind into a molecular structure, the *biexciton*. The situation is completely analogous to hydrogen, the hole playing here the role of the proton : the exciton is the H atom, the biexciton is the H_2 molecule. The molecular binding energy ε_M depends critically on the electron-hole mass ratio $\sigma = m_e/m_h$. While large if $\sigma \ll 1$ (H_2 molecule), ε_M is very small when $\sigma \sim 1$: the hole zero point motion overcomes the additional hole covalent bonding [8]. (Correspondingly, the spatial extent a_M of the biexciton is $\gg a_0$.) Note that these complexes retain spin degrees of freedom : the exciton is singlet or triplet. Among the various biexciton states, the « para » form (electron and hole spin singlets) maximizes the binding (while minimizing the rotational energy).

In actual life, one faces many complications. The gap may be direct or indirect. There may exist several valleys in either the conduction or the valence bands. Bands may be anisotropic — or even orbitally degenerate (as observed in optically active excitons, made up with an s-electron and a p-hole). In addition, the electron and hole spins may be coupled by interband exchange. The resulting many faceted problem is very rich, but very complex. In order to extract simple ideas, it is better to consider first a simple situation (admittedly not realistic) : *a direct gap semiconductor with isotropic, non degenerate bands*. The only parameters are then the density N and the mass ratio σ . Such a model provides the backbone to which we may add, one by one, the above complications.

Consider now a dilute exciton gas, such that $Na_0^3 \ll 1$. If they remain in atomic form, two bound pairs have a small overlap and the excitons can presumably be treated as bosons, whose internal orbital structure is irrelevant. Similarly, a bound biexciton should also behave as a structureless boson if $Na_M^3 \ll 1$. The corresponding ground state presumably breaks some symmetry. One may think of several possibilities :

— *Crystallization* into a regular lattice of either excitons or biexcitons. Crystallization of para-biexcitons has recently been considered by Nikitine [9] : it appears likely if $\sigma \ll 1$ (as in H_2) ; when $\sigma \sim 1$, localizing the holes would probably cost too much kinetic energy.

— *Bose condensation* into a single quantum state with total momentum $q = 0$, as in liquid 4He . Such a possibility has received considerable attention, especially in the work of Hanamura *et al.* [10]. For very dilute systems, $Na_M^3 \ll 1$, the condensed entities

should be biexcitons : one recovers the « pair condensation model » of Bose liquids, which has been sometimes advocated for liquid 4He [13]. As the density increases, biexcitons start overlapping, and eventually they dissociate : we turn into an *atomic exciton condensation* [7] ⁽²⁾.

In what follows, we shall *assume* that the ground state is *Bose condensed*. Such a state, which minimizes the kinetic energy, looks reasonable if $\sigma \sim 1$. In that case, biexciton binding is very weak : we shall ignore it altogether. We thus consider only a *condensate of atomic excitons*. Strictly speaking, that should only hold if

$$a_M^{-3} \ll N \ll a_0^{-3}.$$

Nevertheless, we shall extend the discussion down to $N = 0$.

When $Na_0^3 \gtrsim 1$, the excitons overlap, and one can no longer ignore the fact that the « bosons » are actually made up with two fermions. This is indeed a very old problem [11]. Its impact on the process of Bose condensation was analysed in a pioneering paper by Girardeau [12]. The first terms in a density expansion of the ground state were discussed in detail by Kjeldysh and Kozlov [2] (we shall actually use their approach throughout our paper). Without going into details, a simple argument clearly displays the fundamental physical point. Let a_k^* and b_k^* be creation operators for a conduction and a valence electron, respectively (we temporarily ignore spin). A ground state exciton is characterized by the creation operator

$$\psi_0^* = \sum_k \phi_k a_k^* b_k \quad (1)$$

where $\phi_k \sim 1/a_0^{3/2}$ is the internal orbital wave function. A state with N condensed excitons has a wave function

$$|\Phi_N^0\rangle = \psi_0^{*N} |\text{vac}\rangle \quad (2)$$

($|\text{vac}\rangle$ denotes the intrinsic semiconductor $N = 0$). The corresponding occupancy of the k th fermion state is $n_k = N |\phi_k|^2$. If $Na_0^3 \ll 1$, n_k is $\ll 1$ and we need not worry with the exclusion principle. If however $Na_0^3 \gtrsim 1$, n_k saturates (it cannot exceed 1) : the nature of the bound state changes drastically. Such a saturation is a consequence of the *exchange* between electrons (and holes). Physically, the exciton bound states draw on the same stock of underlying Fermi states ; once that stock is exhausted ($n_k \sim 1$), exchange becomes the dominant feature.

⁽²⁾ The dissociation of biexcitons when N increases was stressed by Brinkman and Rice [5]. They assume it occurs when $N^{-1/3} \sim a_B$, the scattering length of two biexcitons. In practice, the Van der Waals attraction is negligible, and a_B is controlled by the exchange repulsion, $\sim 7 a_0$. Their mechanism is somewhat different from that of reference [7], where dissociation occurs even for point bosons.

We may then approach the problem from the other end, considering a dense system such that $Na_0^3 \gg 1$. The excitons overlap so much that they lose their identity completely. One has better think in terms of an electron-hole plasma. Such a « normal » phase may still be subject to instabilities :

— *Charge density waves* [14] represent the dense counterpart of the crystallized state described in the dilute limit.

— *Excitonic insulator states* may be viewed as Bose condensation of weakly bound electron-hole « Cooper pairs », in much the same way as electron Cooper pairs condense in superconductors. In different guise these states were predicted long ago by Des Cloizeaux [5], by Kozlov and Maksimov [3], the most important contributions being those of Kjeldysh and Kopaeu [1] and of Kohn and co-workers [4]. (Related models were discussed recently in connection with a two band description of rare earth alloys [15].) Such states are known to depend very much on the nature of the gap, on anisotropies and impurity scattering. For our isotropic simplified model, they occur at arbitrarily large density N .

As noted earlier, symmetry breaking is the same in dilute and dense systems. Consequently, one should proceed *smoothly* from one limit to the other, with a gradual change of the physical picture as the density increases : bound pairs which were real atomic entities evolve toward the loose cooperative binding typical of superconductors, a point recently emphasized by Leggett [16] in a somewhat different language.

In an electron gas, we need not worry about possible liquid-gas phase transitions : the density of the system is fixed by the positive charge rigid background. In an electron-hole system, instead, nothing opposes spontaneous density fluctuations (the carriers are globally neutral) : this is just the issue of the electron-hole droplet condensation. The stability of the ground state is controlled by the curve that gives the energy per particle, E_0/N in terms of the volume V/N . Typical situations are shown on figure 1. Original treatments of that problem relied on a comparison of the *normal* plasma with the individual exciton energy ε_0 , with no attempt at describing the intermediate density regime [5]. The consensus was that case « b » would hold for an isotropic semiconductor, band structure effects leading instead to the physically interesting case « c » observed in Ge and Si. We shall see that pairing effects might modify that conclusion (see for instance [6]).

The present paper is concerned only with the direct gap, isotropic non degenerate model defined earlier ; moreover, we completely ignore the spin degrees of freedom of electrons and holes in order to simplify the algebra. We limit ourselves to a *mean field approach*, similar to the BCS theory of superconductivity, using an *unscreened* Coulomb interaction between free carriers. In section 2, we construct the Kjeldysh wave function which describes the Bose condensed

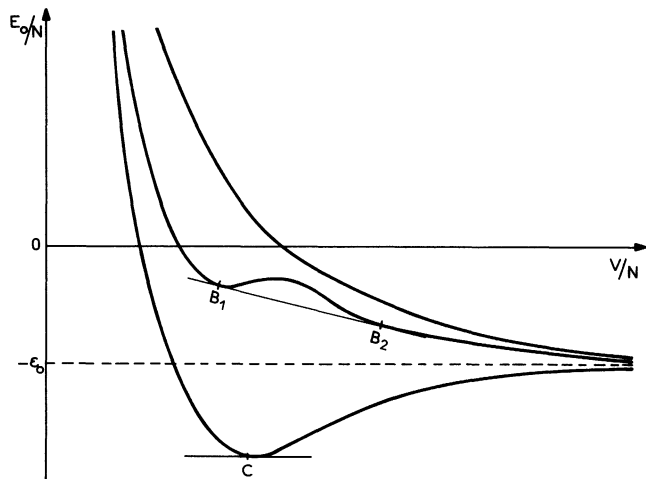


Fig. 1. — Various possibilities for the liquid-gas phase diagram of an electron-hole system. In the dilute limit, the energy per particle goes to the exciton binding energy ($-\varepsilon_0$); case (a) : the homogeneous state is stable at any density; case (b) : liquid gas equilibrium corresponds to the double tangent $B_1 B_2$, i.e. to a finite pressure at $T = 0$; case (c) : the vapour pressure vanishes and the liquid phase has a density corresponding to the minimum C.

ground state for arbitrary density. We consider in detail the dilute and dense limits, where analytic expansions are possible. The nature of elementary excitations is briefly discussed, as well as the critical temperature, whose origin is quite different in the two limits. Section 3 is devoted to a numerical discussion of the intermediate density region. Using the Kjeldysh wave function as a variational ansatz, we interpolate between dense and dilute systems; we show that even at « metallic » densities, pairing corrections are very important.

In a second paper, we shall try to improve on that very crude unrealistic model. First of all, we shall restore the spin degrees of freedom of electrons and holes : *within a mean field approximation*, results are not changed much. Next, we shall examine the effect of screening — a much harder problem for which we can only give estimates. Formally, one can construct a generalized RPA which reduces to the standard treatment of correlations for dense systems [5], and which provides an approximate form of the Van der Waals attraction in the dilute limit. Interpolation at intermediate densities is unfortunately a formidable numerical task, and we shall only present crude, indicative estimates. Finally, we shall briefly survey complications brought about in more realistic models : anisotropies, degenerate bands, multivalley structures, etc...

The problem of the ground state of an electron-hole gas in a semiconductor is extremely rich and diversified : here we only tackle its simpler features. These two papers should be viewed as mostly methodological : at this stage, comparison with experiment would be unrealistic.

2. The Kjeldysh-Kozlov-Kopaev formulation of Bose condensation. — We consider a direct gap semiconductor : momenta k are measured from the band extrema in the Brillouin zone. We assume isotropic, non degenerate parabolic conduction and valence bands. Let $a_{k\sigma}^*$ and $b_{k\sigma}^*$ be the corresponding creation operators. Taking the intrinsic semiconductor as a reference (no free carriers), we write the one electron hamiltonian as

$$H_0 = \frac{\hbar^2 k^2}{2 m_e} a_{k\sigma}^* a_{k\sigma} + \frac{\hbar^2 k^2}{2 m_h} b_{k\sigma}^* b_{k\sigma} . \quad (3)$$

In each band energies are measured from the corresponding extremum ; m_e and m_h are the electron and hole effective masses.

In the Coulomb interaction, we retain only the part associated with *free carriers* : everything connected with the filled valence band is included in either exchange corrections to the gap or in screening by the static dielectric constant κ of the intrinsic material. Moreover, we ignore *interband* electron-hole exchange, involving band to band matrix elements of the density fluctuation ρ_q : the corresponding matrix elements are $\sim q$: they are negligible if the concentration of free carriers is small. (Later, we shall return to these interband terms, as they are the only ones that couple the electron and hole spins.) The Coulomb interaction operator is thus written as

$$H_c = \frac{1}{2} V_q [\rho_q \rho_{-q} - N_e - N_h] \quad (4)$$

in which ρ_q and V_q refer to free carriers only ⁽³⁾

$$\begin{aligned} \rho_q &= a_{k+q,\sigma}^* a_{k\sigma} - b_{k-q,\sigma}^* b_{k\sigma} \\ V_q &= 4 \pi e^2 / \kappa q^2 \end{aligned} \quad (5)$$

N_e and N_h are the number of carriers of each type. The corresponding terms in (4) subtract the self interaction of electrons and holes — equivalently, they act to move the a^* and the b to the left in the product operator $\rho_q \rho_{-q}$.

We fix the free carrier density $N_e = N_h = N$: electrons and holes have each their own chemical potential, μ_e and μ_h (note that μ_h refers to a *hole*, not to a valence electron). The chemical potential for a pair is

$$\mu_e + \mu_h = \mu . \quad (6)$$

Such a canonical description is appropriate if we control the pumping mechanism. If instead electrons and holes exist in thermal equilibrium, μ_e and μ_h are locked by the chemical equilibrium condition

$$\mu_e = G - \mu_h \quad (7)$$

⁽³⁾ Strictly speaking, the intraband matrix element of ρ_q is only 1 if $q \rightarrow 0$: that condition is met for small densities.

where G is the energy gap (absolute Fermi levels are the same in both bands). To the extent that $\mu(N)$ is monotonous, the two points of view are equivalent.

The ground state of a single exciton is hydrogenic. It has a Bohr radius $a_0 = \hbar^2 \kappa / m^* e^2$, where m^* is the reduced mass ($m^{*-1} = m_e^{-1} + m_h^{-1}$). The corresponding « Rydberg » is $\varepsilon_0 = e^2 / 2 \kappa a_0$. Very often, we shall measure k in units $1/a_0$ and energies in units ε_0 , a choice which implies $\hbar^2 / 2 m^* = e^2 / 2 \kappa = 1$. The normalized internal wave function of the $q = 0$ ground state is then

$$\phi_{k0} = \frac{\sqrt{64 \pi}}{(1 + k^2)^2} . \quad (8)$$

The exciton may exist in spin singlet or triplet varieties, whose degeneracy is only lifted by interband exchange. For the moment, we ignore that feature and we simply forget about spin.

Consider now a Bose condensed system of N excitons. At *small densities*, $N a_0^3 \ll 1$, their internal structure is not much affected by neighbours : it should remain close to the single exciton form [8]. If Bose condensation were only macroscopic occupancy of the $q = 0$ exciton state, the corresponding wave function would be (2). Actually, we know that Bose condensation also implies phase locking and large fluctuations in the number of particles. Within a mean field approximation (zeroth order in the Bogoliubov weak coupling expansion), the ground state wave functions should be instead

$$|\Phi_\lambda^0\rangle = e^{\lambda \psi_0^*} |\text{vac}\rangle \quad (9)$$

(within a normalization factor). The modulus of λ fixes the average number of particles ; its arbitrary phase signals the breakdown of gauge invariance. Replacing ψ_0^* by its expression (1), we cast (9) in the form

$$|\Phi_\lambda^0\rangle = \prod_k e^{\lambda \phi_k a_k^* b_k} |\text{vac}\rangle . \quad (10)$$

Finally, we expand the exponential and we remember that electrons and holes are fermions subject to the exclusion principle :

$$|\Phi_\lambda^0\rangle = \prod_k [1 + \lambda \phi_k a_k^* b_k] |\text{vac}\rangle . \quad (11)$$

Upon normalization, (11) appears as a special case of the BCS-like ansatz

$$|\Phi_\lambda^0\rangle = \prod_k [u_k + v_k a_k^* b_k] |\text{vac}\rangle \quad (12)$$

in which

$$\begin{aligned} u_k &= \frac{1}{\sqrt{1 + |\lambda \phi_k|^2}} \approx 1 , \\ v_k &= \frac{\lambda \phi_k}{\sqrt{1 + |\lambda \phi_k|^2}} \approx \lambda \phi_k \ll 1 . \end{aligned} \quad (13)$$

The fact that (12) can describe *Bose condensation of dilute excitons* was recognized by Kjeldysh and Kozlov [2] : the shape of v_k then depicts the internal state of the bound electron hole pair, while its magnitude, $\lambda = \sqrt{N}$, fixes the density. The corresponding behaviour of $|v_k|^2$ as a function of $\varepsilon_k = \hbar^2 k^2/2 m^*$ is sketched on figure 2.

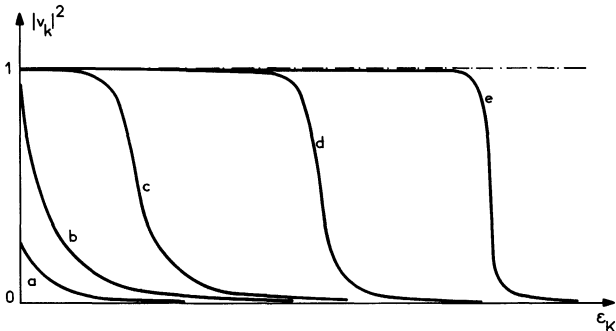


Fig. 2. — The ground state fermion distribution $(v_k)^2$, as a function of pair energy ε_k for various densities N . Curves (a) and (b) correspond to dilute systems ($Na_0^3 \ll 1$), in which $(v_k)^2$ scales with a constant shape as a function of N . Curves (d) and (e) correspond to the dense limit : the Fermi level drop sharpens and moves to higher energies. The transition between these two limits is smooth, as shown by curve (c).

Let us follow the evolution of (12) as the pair density N grows. $|v_k|^2$ first increases in magnitude without changing its shape. When $|v_k|^2$ approaches 1, it is « stopped » by the normalization condition $|u|^2 + |v|^2 = 1$ — a mathematical statement of the exclusion principle. Physically, the N condensed excitons exhaust the underlying stock of fermion states. In order to pack up more particles, v_k must spread further away in k -space. Since $\phi_k \sim a_0^{-3/2}$, such a saturation occurs when $Na_0^3 \sim 1$, i.e. when excitons start overlapping.

We may also start from the opposite end, $Na_0^3 \gg 1$. The ansatz (12) describes equally well the usual degenerate electron-hole plasma : we need only take for $|v_k|^2$ a step function

$$|v_k|^2 = \begin{cases} 1 & \text{if } k < k_F \\ 0 & \text{if } k > k_F \end{cases} \quad (14)$$

where $k_F = (6\pi^2 N)^{1/3}$ is the Fermi wave vector (remember we ignore spin !). As a function of ε_k , the distribution levels off at the pair chemical potential $\mu_e + \mu_h = \mu$. Actually (14) is only a first approximation. As shown by Kjeldysh-Kopaev and by Kohn [4], however large the density (and small the interaction), an *isotropic* electron-hole gas always undergoes an instability analogous to superconductivity — except that electron pairs become electron-hole pairs. The resulting *excitonic* insulator is still described by (12), except that $|v_k|^2$ is rounded off near $\varepsilon_k = \mu$, over a width Δ that decreases exponentially when N grows. Δ is the energy gap.

Putting the two limits together, we see that the Kjeldysh wave function provides a smooth transition between the dilute condensed excitons in one limit, the excitonic insulator and ultimately the electron-hole plasma in the other. The evolution of $|v_k|^2$ as the density increases is sketched on figure 2 : when saturation is reached, $|v_k|^2$ extends to larger energies ε_k , with a sharper and sharper drop. Since (12) accurately describes the limits $N \rightarrow 0$ and $N \rightarrow \infty$, it may be viewed as an *interpolation* in the intermediate density region, which cannot be very wrong. Mathematically, it is simple — however the physical interpretation is no longer obvious : curve c in figure 2 is equally remote from condensed point bosons (curves a and b) and from a degenerate plasma (curves d and e).

In our isotropic model, Bose condensation occurs at all densities. As a result, the ground state is always an insulator. One always can think in terms of bound electron-hole pairs, but with a different physical picture in the two limits. For small N , the pairs are well identified, each electron interacting with only one hole, except for infrequent collisions. For large N , we are dealing with Cooper pairs whose radius is much larger than the particle spacing. Binding is then a cooperative effect rather than a single pair affair.

Actually, (12) is nothing but the *mean field* approximate ground state, taking into account Bogoliubov anomalous pairing $\langle a^* b \rangle$ as well as the ordinary Hartree Fock pairing $\langle a^* a \rangle$ and $\langle b b^* \rangle$. At the moment, we view it as a *variational ansatz* in terms of the unknown v_k , subject to the normalization condition

$$|u_k|^2 + |v_k|^2 = 1 \quad (15)$$

(it provides the best mean field ground state). Since the number of pairs is not conserved, we minimize $\langle H - \mu N \rangle$. Disregarding spin, the corresponding expectation value is

$$F = \langle E - \mu N \rangle = \sum_k (\varepsilon_k - \mu) v_k^2 - \sum_{kk'} V_{k-k'} \times [v_k^2 v_{k'}^2 + u_k u_{k'} v_k v_{k'}] \quad (16)$$

$\varepsilon_k = \hbar^2 k^2/2 m^*$ is the *pair* kinetic energy. The second term is the usual electron-electron and hole-hole exchange (hence the absence of a factor 1/2). There is no Hartree term since the gas is globally neutral. The last term is the *anomalous* interaction due to Bose condensation (as in a superconductor). Note that we must include the normal Fock terms which are often discarded in simple treatments : they control the energy at high densities and they are crucial in the minimization. It is easily shown that (16) is stationary subject to (15) if v_k obeys the following condition

$$\left[\varepsilon_k - \mu - 2 \sum_{k'} V_{k-k'} |v_{k'}|^2 \right] u_k v_k - (u_k^2 - v_k^2) \sum_{k'} V_{k-k'} u_{k'} v_{k'} = 0 \quad (17)$$

(17) is the basic input of our discussion. It is solved by setting ⁽⁴⁾

$$\left. \begin{aligned} \varepsilon_k - \mu - 2 \sum_{k'} V_{k-k'} |v_{k'}|^2 &= \xi_k \\ 2 \sum_{k'} V_{k-k'} u_{k'} v_{k'} &= \Delta_k \\ E_k^2 &= \xi_k^2 + |\Delta_k|^2 \end{aligned} \right\}. \quad (18)$$

Standard algebra then yields

$$\left. \begin{aligned} u_k v_k &= \frac{\Delta_k}{2 E_k} \\ |v_k|^2 &= \frac{1 - \xi_k/E_k}{2} \end{aligned} \right\}. \quad (19)$$

Solved self consistently, (18) and (19) provide the unknown ξ_k and Δ_k . μ is chosen last in such a way as to ensure the required value of $N = \sum |v_k|^2$.

Such a formulation is valid at arbitrary density — but it can be pushed through analytically only in limiting cases. We first consider the dilute limit, analysed in detail by Kjeldysh and Kozlov [2]. v_k is then small and in leading order, (17) reduces to the homogeneous equation

$$(\varepsilon_k - \mu) v_k - \sum_{k'} V_{k-k'} v_{k'} = 0 \quad (20)$$

(20) is nothing but the Schrödinger equation for the single exciton bound state. Normalizing v_k so that $\sum |v_k|^2 = N$, the zeroth order solution is

$$\left. \begin{aligned} \mu &= -\varepsilon_0 \\ v_{k0} &= \sqrt{N} \phi_{k0} \end{aligned} \right\}. \quad (21)$$

As expected, the chemical potential μ is the (negative) energy of a single bound exciton. It appears through a linear eigenvalue equation which also fixes the shape of v_k . In that order, excitons are completely independent, and the density N only enters through the magnitude of v_k . Knowing v_{k0} , we easily infer the condensation parameter Δ_k :

$$\Delta_k = 2 \sum_{k'} V_{k-k'} v_{k'0} = 2(\varepsilon_k + \varepsilon_0) \phi_{k0}^0 \sqrt{N}. \quad (22)$$

It vanishes when $N \rightarrow 0$ (contrary to μ).

Proceeding to the next order in N as in perturbation theory, we write

$$\left. \begin{aligned} v_k &= \alpha \phi_{k0} + \delta v_k \\ \mu &= -\varepsilon_0 + \delta \mu \end{aligned} \right\} \quad (23)$$

with δv_k orthogonal to ϕ_{k0} . To first order in δv_k , (17) reduces to

$$\left. \begin{aligned} (\varepsilon_k + \varepsilon_0) \delta v_k - V_{k-k'} \delta v_{k'} &= -\lambda_k + \alpha \phi_{k0} \delta \mu \\ \lambda_k &= \frac{\alpha^3}{2} V_{k-k'} \phi_{k'0} [3 \phi_{k0}^2 - 4 \phi_{k0} \phi_{k'0} + \phi_{k'0}^2] \end{aligned} \right\} \quad (24)$$

δv_k is $\sim \alpha^3$ and therefore $N = \alpha^2 + 0(\alpha^6)$. On projecting the first equation (24) onto ϕ_{k0} , we obtain (see Appendix A)

$$\delta \mu = \frac{1}{\alpha} \sum_k \lambda_k \phi_{k0} = \frac{26 \pi}{3} N a_0^3 \varepsilon_0 \quad (25)$$

(25) is the lowest order correction to the chemical potential, first derived by Kjeldysh and Kozlov [2]. It arises from the exchange *repulsion* between the electrons and the holes that make the interacting excitons — hence its positive sign. Such a short range repulsion due to overlap of internal wave functions is familiar. What is unusual is how simply it enters the formalism — though a saturation of the coefficient v_k^2 : that is a consequence of the Bose condensation.

Actually, (25) is not the only contribution of order N in the dilute limit. Besides the static repulsion due to the exclusion principle, two excitons should feel an *attraction* due to their joint virtual excitation; at large distances, it becomes the usual Van der Waals potential. The existence of that other contribution to $\delta \mu$ was also recognized by Kjeldysh and Kozlov, who gave its complete formal expression; we shall see that such an attraction may be viewed as the dilute limit of *screening* corrections.

In next order, $\delta \mu \sim N^2$, the mean field approximation breaks down completely (it already failed to provide the attraction in order N). This is well known for an ordinary Bose gas of point particles (17). We nevertheless carry the solution of (17) one step further in Appendix A: the calculation has no real physical significance, but it provides a test for crude numerical solutions of (17).

An explicit solution is equally straightforward in the high density limit, $N a_0^3 \gg 1$. In zeroth order, Δ vanishes and the system is an ordinary Hartree Fock plasma (the density fixes k_F , and the chemical potential is in turn the Fermi energy ε_F). In next order, a small excitonic insulator instability develops. With logarithmic accuracy, we can take Δ_k constant: we just need to minimize (16) with respect to Δ . For a short range interaction, we would find

$$F - F_0 = \frac{1}{2} N_0 \Delta^2 \log \frac{E_c}{\Delta} - N_0^2 V \Delta^2 \left(\log \frac{E_c}{\Delta} \right)^2$$

in which E_c is a cut off of order ε_F , V is the angular average of $V_{kk'}$ over the Fermi surface and N_0 is the density of states at Fermi level ⁽⁵⁾. Minimization yields the usual BCS weak coupling result:

$$\Delta = E_c \exp \left[-\frac{1}{2 N_0 V} \right]. \quad (26)$$

⁽⁴⁾ Note that Δ_k , E_k are here *pair* energies. As compared to the usual quasiparticle description E_k is the energy needed to create an electron *and* a hole with equal momenta k . Similarly, Δ_k is a *pair* gap, twice the usual BCS gap. Such a formulation is more convenient in our variational approach.

⁽⁵⁾ N_0 is defined with respect to the *pair* energy: hence the factor 2 in (26).

Strictly speaking, (26) is not valid here because we use a long range unscreened Coulomb interaction. As a result, an additional singularity appears when $k \rightarrow k'$. Within our constant Δ ansatz, we find easily that

$$F - F_0 = \frac{1}{2} N_0 \Delta^2 \log \frac{E_c}{\Delta} - \frac{2 \pi e^2}{3 k_F^2} N_0^2 \Delta^2 \left(\log \frac{E_c}{\Delta} \right)^3$$

which upon minimization gives

$$\Delta = E_c \exp \left[- \frac{1}{\sqrt{4 \pi e^2 N_0 / 3 k_F^2}} \right] \quad (27)$$

(27) is useful as a test of our interpolation scheme : in real life, it is unphysical since the interaction is always screened ! We should retain only one conclusion ; the gap vanishes exponentially when the density N goes to ∞ .

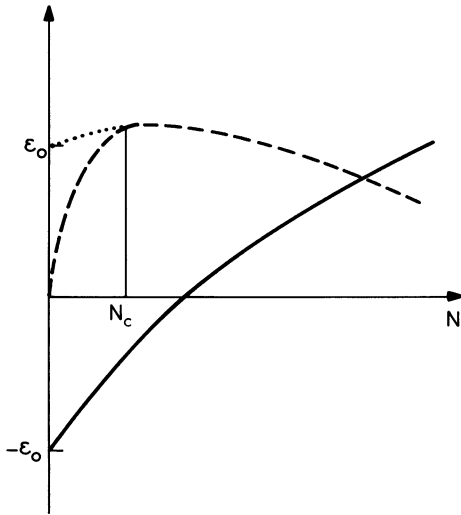


Fig. 3. — A rough sketch of the behaviour of μ (full curve), Δ (dashed curve) and E_m (dashed curve when $N > N_c$, dotted curve when $N < N_c$) as a function of density N .

We show in figure 3 a possible interpolation of the various parameters in the intermediate density region. We may define an « effective » order parameter $\Delta = \Delta(k_F)$, where $k_F = (6 \pi^2 N)^{1/3}$ is the Fermi wave vector of non interacting electrons and holes. Δ vanishes in both limits, going through a maximum in between. The chemical potential μ is $\sim -\epsilon_0$ at small density, while it is positive for large N ($\sim$ the Fermi energy). In figure 3, we assumed $\mu(N)$ was monotonous, a conclusion which is supported by the numerical analysis of section 3.

E_k represents the energy needed in order to create an electron-hole pair, each with momentum k (it corresponds to *ionization* of a condensed bound pair). The minimum value of E_k is the actual *energy gap* E_m for such excitations. From (18), we may write

$$\left. \begin{aligned} E_k &= [(\epsilon_k - \tilde{\mu}_k)^2 + \Delta_k^2]^{1/2} \\ \tilde{\mu}_k &= \mu + 2 \sum_{k'} V_{k-k'} |v_{k'}|^2 \end{aligned} \right\} \quad (28)$$

When $\tilde{\mu}_k$ is > 0 , the minimum value of E_k is achieved when $\epsilon_k - \tilde{\mu}_k = 0$: the energy gap is then Δ ⁽⁶⁾. Such a case, characteristic of usual superconductors, holds at large densities. If however $\tilde{\mu}_k$ is < 0 , the minimum E_k corresponds to $\epsilon_k = 0$, i.e. to the zone centre, as pointed out by Leggett [16]. The energy gap is then

$$E_m = \sqrt{\tilde{\mu}_0^2 + \Delta_0^2}. \quad (29)$$

In the extreme dilute limit, E_m goes to ϵ_0 , the free exciton binding energy — as expected. We can in fact push the calculation one step further. For small N , Δ_k is given by (22). Similarly, using the machinery of Appendix A, we find that

$$\tilde{\mu}_k = \mu + 128 \pi N a_0^3 \epsilon_0 I_4(ka_0) \quad (30)$$

(see (A.6) and (A.7)). Using (25), we thus obtain

$$E_m = \epsilon_0 \left[1 + \frac{118 \pi N a_0^3}{3} \right]. \quad (31)$$

Starting from the dilute limit, the energy gap first *increases*, despite the fact that $|\mu|$ decreases : the order parameter Δ_0 supersedes the decrease of $|\tilde{\mu}_0|$. Eventually, E_m will go through a maximum. The qualitative behaviour of $E_m(N)$ is also sketched on figure 3 : the energy gap changes smoothly from a small cooperative effect in the dense limit into a strictly *atomic* quantity in the dilute case.

In addition to the quasiparticle excitations, the ground state (9) possesses *collective* excitations, that can be viewed either as a bound quasiparticle pair or as fluctuations of the order parameter $\langle a_k^* b_k \rangle$. In the dense limit, these are the Bogoliubov modes inside the gap Δ ; in the opposite dilute case, they are the « phonons and rotons » of our Bose gas, describing *centre of mass motion* of the *bound* excitons (as opposed to ionized quasiparticles). Once again, one goes smoothly from one to the other as N varies.

An important parameter is the critical temperature T_c at which Bose condensation disappears. Unfortunately, the Kjelldysh approach does not permit a smooth description of T_c throughout the whole density range, as it does for the ground state. Basically, (9) is a mean field approximation, which only describes bound pairs with total $q = 0$: it does not account for thermal excitation of collective modes — corresponding to the « normal », uncondensed fluid in liquid ⁴He language. This is not important in the dense limit, where thermodynamics is controlled by *ionization* of excitons : T_c then results from breaking of condensed pairs, a process which is easily incorporated in the BCS-type formulation. On the contrary, ionization is negligible in the dilute limit : only the centre of mass excitation of *bound* excitons is relevant ; T_c is reached

⁽⁶⁾ That minimum may be slightly shifted if we take into account the k -dependence of Δ_k .

when the $q = 0$ state is empty, a process that no mean field calculation can account for.

For large N , T_c is exponentially small, of order Δ . In the other limit $N \rightarrow 0$, we recover a free Bose gas, in which $T_c \sim N^{2/3}$. In between, T_c should go through a maximum, which we do not know how to calculate. It is not even clear whether the evolution is smooth; the transition temperature might result from different mathematical singularities in both cases. If we start from the normal high temperature state, we expect a singularity to develop

— when the electron-hole t -matrix at the Fermi level diverges : this is the Thouless [18] criterion for critical temperature in a superconductor ;

— when the chemical potential μ reaches the bottom of the bound state exciton band ; that provides the T_c of a free Bose gas.

It is not clear whether these two singularities are manifestations of one and the same thing. If they are not, T_c should display a cusp at intermediate N , when the two critical temperatures cross (Fig. 4). More likely, the instability changes its nature progressively, and T_c is smooth.

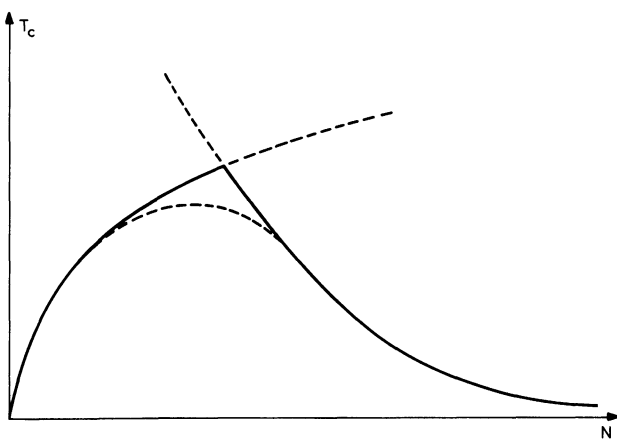


Fig. 4. — The critical temperature T_c for Bose condensation as a function of N (a) if there exist two distinct instability mechanisms (full curve) (b) if only one instability changes its nature progressively (dashed curve).

3. Numerical interpolation in the intermediate density region. — Our variational ansatz (12) can be used for arbitrary densities. In principle, we could use it directly, and minimize the general expression (16) as a function of v_k — either by solving the non linear equation (17) or by direct Monte Carlo minimization. The numerical work, however, is rather formidable, not really worth the effort in view of the crude, oversimplified model we are using. We shall thus limit our ambitions : we shall take for v_k a simple functional form, depending only on two parameters, and we shall minimize the energy with respect to these parameters. Our calculation may be viewed as an interpolation between the dense and dilute limits — not the best

variational choice for v_k , yet one which is reasonable. Similar calculations were made long ago by Silin and by Zimmermann [6], using a rather crude choice for v_k . We wish here to be more realistic — at the expense of numerical computation ; we shall choose a shape of v_k which is correct in the two limits $N \rightarrow 0$ and $N \rightarrow \infty$.

From (19), we see that

$$\lambda_k = \frac{u_k v_k}{u_k^2 - v_k^2} = \frac{\Delta_k}{2 \xi_k} \quad (32)$$

(2 $\lambda_k = \tan 2 \theta_k$ yields the « angle » θ_k of the Bogoliubov canonical transformation). In the dilute limit, v_k is $\ll 1$ and

$$\lambda_k \approx \sqrt{N} \psi_{k0} = \frac{\sqrt{64 \pi N}}{(1 + k^2)^2} \quad (33a)$$

(we now use the reduced units defined earlier). In the opposite dense limit, Δ is small and we have

$$\lambda_k \approx \frac{\Delta}{2[k^2 - k_F^2]}. \quad (33b)$$

In between, we try an interpolation which reduces to the right limits :

$$\lambda_k = \frac{\zeta}{(1 + k^2)(k^2 - \Omega)} \quad (34)$$

ζ and Ω are our new variational parameters. When $N \rightarrow 0$, we expect that $\zeta \rightarrow 0$, $\Omega \rightarrow -1$; if instead $N \rightarrow \infty$, ζ should again vanish while $\Omega \sim k_F^2$ (thereby restoring electron-hole symmetry around the Fermi level).

The numerical calculation is then straightforward, although fairly heavy. From (34) we infer v_k , which we carry into (16). We then do the integration numerically in order to obtain

$$\langle E \rangle = f(\zeta, \Omega), \quad \langle N \rangle = g(\zeta, \Omega).$$

Each density N corresponds to a curve in the (ζ, Ω) plane : we minimize $\langle E \rangle$ along that curve. Altogether, we only use *one* parameter in order to characterize the *shape* of v_k : the other parameter is actually the density.

In figure 5, we show our results for the energy per particle, ε . The density is measured by the interparticle spacing r_s , defined as ⁽⁷⁾

$$\frac{4 \pi r_s^3}{3} = \frac{1}{N} \quad (35)$$

(remember that $\varepsilon_0 = a_0 = 1$). On the same figure, we plot the result of a standard Hartree Fock calculation

$$\varepsilon_{\text{HF}} = \frac{3}{5} \left(\frac{9 \pi}{2 r_s} \right)^{2/3} - \frac{3}{\pi} \left(\frac{9 \pi}{2 r_s} \right)^{1/3} = \frac{3.15}{r_s^2} - \frac{2.31}{r_s}. \quad (36)$$

⁽⁷⁾ Here we do not include spin degeneracy : our definition of r_s differs from the usual one by a factor $2^{1/3}$.

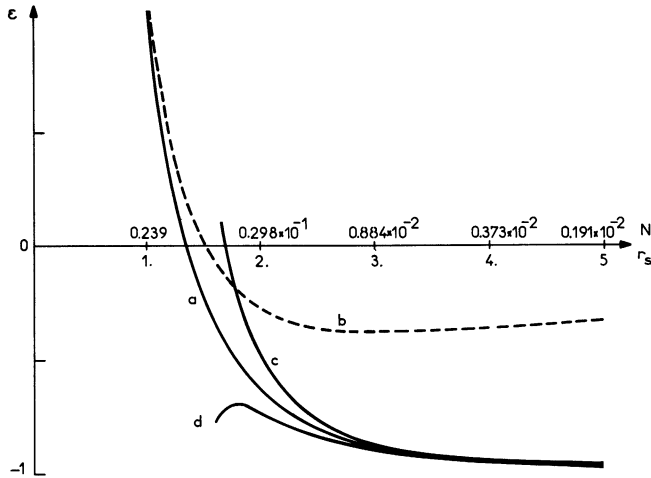


Fig. 5. — The ground state energy per particle, ε , as a function of interparticle spacing, r_s , defined in (31). Energies are measured in units ε_0 , r_s in units a_0 . Curve « a » is the result of our variational interpolation ansatz (30). Curve « b » is the usual Hartree Fock ground state energy, given by (32). Curves « c » and « d » correspond to the low density expansions of appendix A, respectively within the heuristic ansatz (30) and from the exact expression (17) of the ground state energy.

Note that the Hartree Fock ground state is a special case of our variational ansatz (12), corresponding to a step function $v(\varepsilon_k)$: ε_{HF} is thus above the real ε , as verified by numerical calculation. That result calls for a number of comments :

(i) ε goes smoothly from the Hartree Fock energy at high density into the single exciton energy $-\varepsilon_0 = -1$ when $r_s \rightarrow \infty$. Such a feature, already obtained by Silin [6], is a definite improvement on older treatments of Coulomb interactions, which did not take into account the tendency to form bound pairs. Here, *because of Bose condensation*, we can follow the transition smoothly from one end to the other.

(ii) The curve $\varepsilon(r_s)$ is monotonous : there is no liquid gas phase separation. In fact, that result is probably specific of our simple model. We shall see later that a crude treatment of screening seems to restore a first order transition. Anyhow, degenerate or anisotropic bands will make pairing harder as N increases : that may restore the Hartree Fock minimum.

(iii) The minimum of ε_{HF} , occurring at $r_s \sim 3$, corresponds to so called « metallic densities ». We see that at such densities, ε is over twice ε_{HF} . The pairing corrections, describing the progressive formation of bound excitons, are thus extremely important. That fact is well known to nuclear theorists, who have included such pairing terms in their nuclear models for a long time. The physical effect is may be more transparent here, emerging as it does from the formation of a bound state. In any case, it is clear that any calculation that ignores pairing is questionable. (The situation is completely different for the usual one

component plasma, in which there is no attractive force.)

(iv) In order to assess the validity of our restricted variational ansatz (34), we also plot in figure 5 the result of a direct density expansion in the dilute limit, carried out in Appendix A. Curve « c » is the expansion within the ansatz (34), curve « d » is the exact expansion of the general equation (17). We see that the agreement is quite good in the range of convergence of such expansions.

The behaviour of $\varepsilon(r_s)$ is just what one would guess knowing the expansions in the two limits of small and large densities. Indeed, if we were to draw the curve of figure 5 « with the artist's touch », there would be little freedom ! It is nevertheless gratifying to have a quantitative interpolation scheme based on a well defined ansatz.

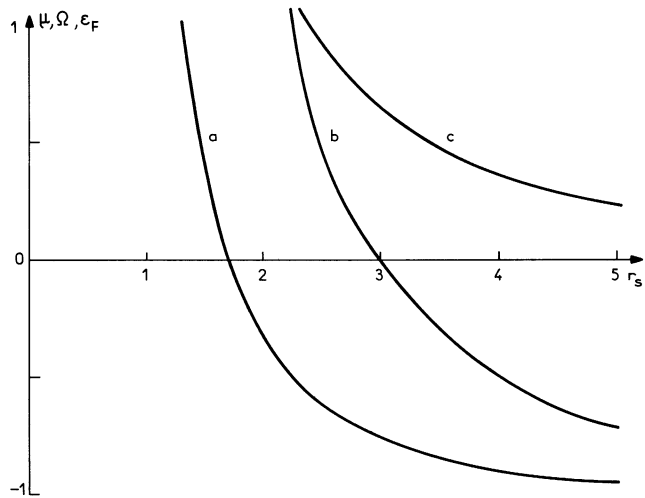


Fig. 6. — The chemical potential μ as a function of r_s (curve « a »), as compared to the variational parameter Ω (curve « b »), and to the Fermi energy ε_F of a free particle gas with the same density (curve « c »).

We may analyse our result further. In figure 6, we plot the chemical potential μ as a function of r_s , as well as the parameter Ω of our variational ansatz, and the Fermi energy $\varepsilon_F = \hbar^2 k_F^2 / 2 m^*$ of a non interacting gas with the same density ($N = k_F^3 / 6 \pi^2$). In the dilute limit $|r_s \rightarrow \infty|$, μ and Ω go to the same limit -1 , but with a different slope (see (A.17)). In the other limit $r_s \rightarrow 0$, μ and Ω should both reduce to the same value ε_F : however, we are still far from that limit when $r_s \sim 1$. In that region, Ω is already very close to ε_F : the transition region in which v_k drops from 1 to 0 is nearly centred on the Fermi energy (as it would be in an ordinary superconductor). Put another way, the excitonic insulator instability does not affect much electron-hole symmetry. On the other hand, $\mu \ll \Omega$, a feature which signals the importance of interaction terms in the energy.

The order parameter Δ_k is given by (18) : using our

ansatz (34), we can calculate it numerically. The corresponding k -dependence is sketched on figure 7 for various densities. For small N , we have

$$\Delta_k \sim \frac{2\zeta}{1+k^2}$$

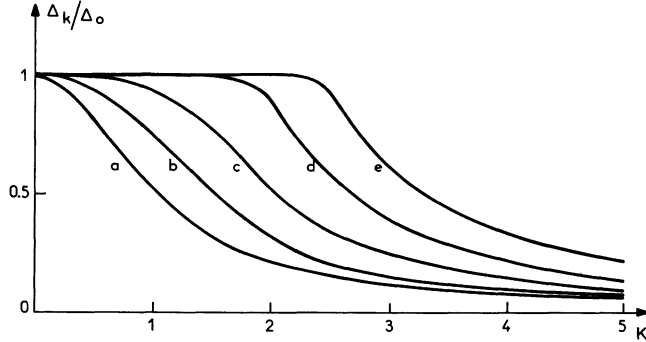


Fig. 7. — The relative order parameter, Δ_k/Δ_0 , as a function of momentum k , for various densities : « a » : $r_s = 10$; « b » : $r_s = 3$; « c » : $r_s = 1.75$; « d » : $r_s = 1.3$; « e » : $r_s = 1$.

(see (22)). When N grows, Δ extends to larger k ; at first it shows a flat plateau. Ultimately, it should develop a logarithmic peak near k_F , due to the long range of the bare Coulomb interaction. If we perform the angular integration in (18), we find

$$\Delta_k = \frac{2}{\pi k} \int_0^\infty k' dk' \operatorname{Ln} \left| \frac{k+k'}{k-k'} \right| u_{k'} v_{k'}.$$

The narrower the profile of $u_{k'} v_{k'}$, the stronger the peak at $k = k_F$. Such a singularity is related to the unusual behaviour (27) : it would be strongly reduced if we included screening. Anyhow, it does not show up yet at $r_s = 1$ (the gap is still too large and it blurs the logarithm). In practice, we can by pass the difficulty by calculating Δ at the Fermi level directly from (28) instead of (18). If we ignore the k -dependence of the Fock term (which is small at high density), we see that

$$\lambda_k \sim \frac{\Delta}{2(k^2 - k_F^2)} \sim \frac{\zeta}{(1 + k_F^2)(k^2 - k_F^2)}.$$

It follows that

$$\Delta \sim \Delta^* = \frac{2\zeta}{1 + k_F^2}. \quad (37)$$

In practice Δ^* is a useful characterization of the order parameter which is always very close to the effective $\Delta = \Delta(k_F)$ defined earlier. In figure 8, we plot the density variation of Δ^* (which also specifies completely our variational parameters), as well as the numerical values of Δ and of the $k = 0$ value, Δ_0 . The maximum is clearly apparent.

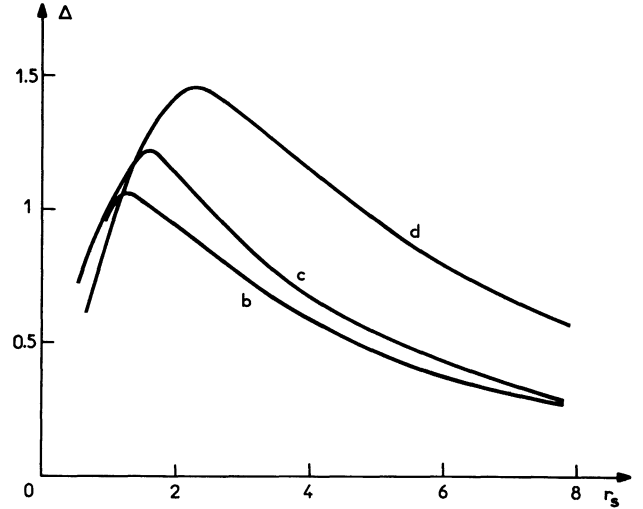


Fig. 8. — The parameter $\Delta^* = 2\zeta/(1 + k_F^2)$ as a function of r_s (curve « d »). For comparison, we also plot the numerical value of $\Delta = \Delta(k_F)$ (curve « b ») and of $\Delta_0 = \Delta(0)$ (curve « c »).

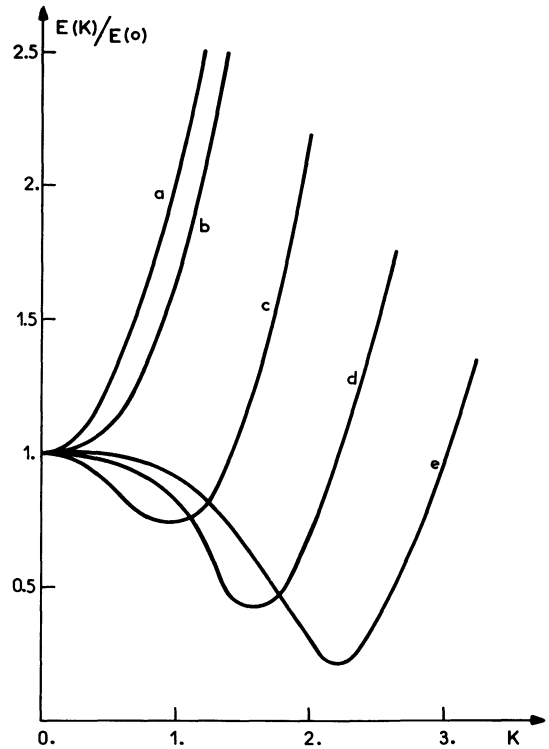


Fig. 9. — The pair excitation energy E_k as a function of k for various densities (the same as in figure 7).

Finally, we show in figure 9 the behaviour of the excitation energy E_k as a function of k for various densities. As described qualitatively in section 2, the minimum of E_k , located at $k = 0$ when N is small, moves out to finite k at larger density. The variation of E_m as a function of density is plotted in figure 10,

together with the momentum at which the minimum occurs. Numerical interpolation thus substantiates guesses of the preceding section.

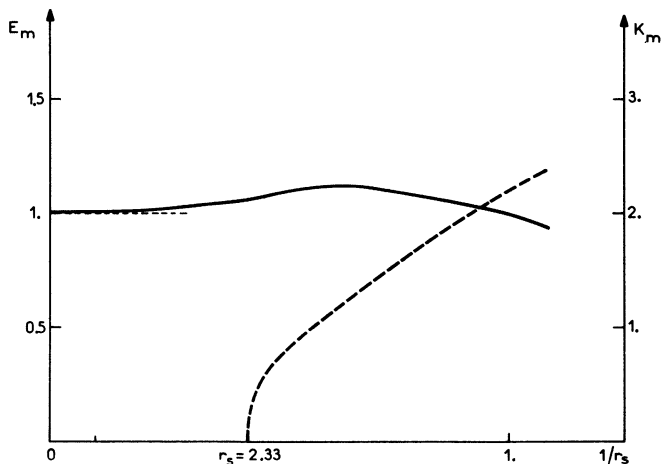


Fig. 10. — The minimum energy E_m (full curve) and the momentum k_m at which it occurs (dashed curve) as a function of $1/r_s$.

4. Conclusion. — We have shown how a BCS-like mean field wave function can describe the transition between dilute excitons and a dense electron-hole plasma. This is made possible by Bose condensation which guarantees that all bound pairs have the same total momentum $q = 0$. As a result, the tendency to form bound pairs can be incorporated into an order parameter — as it is commonly done in nuclei. We find that the ground state energy goes smoothly from the Hartree Fock value to the free exciton energy $-\varepsilon_0$. Within our variational ansatz, and for our simple isotropic band model, there is no liquid-gas phase separation. We shall see in a second paper that such a conclusion is probably invalid if we include screening. We note that pairing corrections are still very important at so called « metallic densities » $r_s \sim 1$ (way beyond the minimum of the Hartree Fock curve).

We discussed the variation of relevant physical quantities as a function of density. The order parameter Δ goes through a maximum, while the energy gap departs from Δ at low density : it goes toward the atomic exciton ionization energy. We briefly discussed the critical temperature, which also vanishes in both limits : we pointed out that the physical origin of T_c was completely different in dilute and dense systems.

Except for a more realistic wave function, our formulation is equivalent to that of Silin and of Zimmermann [6]. We tried to cast it in a very simple variational language that can be readily generalized to more complicated situations.

Acknowledgments. — We are indebted to J. Biellman and M. Simon (L.O.S.C.S., Strasbourg) for their help in performing numerical computations.

Appendix A. — We want to expand the solution of (17) in powers of N . We start from the general expression (16), and we replace u_k by

$$u_k = 1 - \frac{v_k^2}{2} - \frac{v_k^4}{8} + \dots$$

We are thus led to minimize the quantity

$$\langle H - \mu N \rangle = F_0 + F_1 + F_2 + \dots - N\delta\mu \quad (\text{A.1})$$

in which we have set

$$\left. \begin{aligned} F_0 &= (\varepsilon_k + \varepsilon_0) v_k^2 - V_{k-k'} v_k v_{k'} \\ F_1 &= V_{k-k'} \frac{v_k v_{k'}}{2} (v_k - v_{k'})^2 \\ F_2 &= V_{k-k'} \frac{v_k v_{k'}}{8} (v_k^2 - v_{k'}^2)^2 \end{aligned} \right\} \quad (\text{A.2})$$

We write v_k in the form (23)

$$v_k = \alpha \phi_{k0} + \delta v_k \quad (\text{A.3})$$

in which ϕ_{k0} is the normalized ground state exciton wave function (8), δv_k being orthogonal to ϕ_{k0} . The number α and δv_k will both result from the minimization process.

We know that $\alpha \sim \sqrt{N}$; moreover δv_k , given by (24), is of order $\alpha^3 \sim N^{3/2}$. Finally $\delta\mu$ is $\sim N$. Retaining only terms up to order N^3 inclusive in (A.2), we find :

$$\left. \begin{aligned} F_0 &= (\varepsilon_k + \varepsilon_0) \delta v_k^2 - V_{k-k'} \delta v_k \delta v_{k'} \\ F_1 &= A\alpha^4 + 2\lambda_k \delta v_k \\ F_2 &= B\alpha^6 \end{aligned} \right\} \quad (\text{A.4})$$

(remember that $v_{k0} = \alpha \phi_{k0}$ is a solution of (19)). λ_k is exactly the coefficient defined in (24). A and B are numbers,

$$\left\{ \begin{aligned} A &= V_{k-k'} \frac{\phi_{k0} \phi_{k'0}}{2} (\phi_{k0} - \phi_{k'0})^2 \\ B &= V_{k-k'} \frac{\phi_{k0} \phi_{k'0}}{8} (\phi_{k0}^2 - \phi_{k'0}^2)^2. \end{aligned} \right.$$

We shall first minimize (A.1) with respect to δv_k , and then with respect to α . From the resulting α and δv_k , we can infer the total number of particles

$$N = \alpha^2 + \sum_k \delta v_k^2 = \alpha^2 + O(\alpha^6). \quad (\text{A.5})$$

Hence the relationship $\mu(N)$ which is our final goal.

The algebra is straightforward, but somewhat tedious. It is convenient to use reduced units in which $a_0 = \varepsilon_0 = 1$. With that choice

$$\varepsilon_k + \varepsilon_0 = 1 + k^2, \quad \phi_{k0} = \frac{\sqrt{64\pi}}{(1 + k^2)^2},$$

$$V_{k-k'} = \frac{8\pi}{(k - k')^2}.$$

All the calculation uses the following integrals :

$$\begin{aligned}\beta_n &= \int_0^\infty \frac{dk}{(1+k^2)^n} = \frac{\pi}{2} \frac{1 \dots (2n-3)}{2 \dots (2n-2)} \\ S_{mn} &= \sum_{kk'} \frac{V_{k-k'}}{(1+k^2)^m (1+k'^2)^n} = \frac{\beta_m \beta_n}{\pi^3 (n+m-2)} \\ I_m(k) &= \sum_{k'} \frac{V_{k-k'}}{(1+k'^2)^m}.\end{aligned}\quad (\text{A.6})$$

In calculating S_{mn} we do the angular integration first, and we integrate by parts with respect to k and k' . In the same way, we establish the recursion relation

$$I_{m+1} = \frac{(m-1)I_m + 2\beta_m/\pi}{m(1+k^2)}.\quad (\text{A.7})$$

Starting from $I_2 = (1+k^2)^{-1}$, (A.7) yields all the successive I_m . With the help of (A.6), we easily obtain A and B :

$$\begin{aligned}A &= (64\pi)^2 [S_{26} - S_{44}] = \frac{13\pi}{3} \\ B &= \frac{(64\pi)^3}{4} [S_{2,10} - S_{66}] = \frac{4.217\pi^2}{80}.\end{aligned}\quad (\text{A.8})$$

Minimization with respect to δv_k yields an equation similar to (24) :

$$(\varepsilon_k + \varepsilon_0) \delta v_k - V_{k-k'} \delta v_{k'} = -\bar{\lambda}_k \quad (\text{A.9})$$

where $\bar{\lambda}_k$ is the part of λ_k orthogonal to ϕ_{k0} . Using (A.7), we may calculate it explicitly :

$$\left\{ \begin{aligned} \bar{\lambda}_k &= (64\pi)^{3/2} \alpha^3 \sum_{m=1}^5 \frac{\beta_m}{(1+k^2)^m} \\ \beta_5 &= \frac{14}{15}, \quad \beta_4 = -\frac{17}{60}, \quad \beta_3 = -\frac{17}{80}, \\ \beta_2 &= -\frac{5}{48}, \quad \beta_1 = \frac{7}{256}. \end{aligned} \right.$$

It turns out that (A.9) can be solved explicitly in the following form :

$$\left\{ \begin{aligned} \delta v_k &= (64\pi)^{3/2} \alpha^3 \sum_{m=2}^6 \frac{\gamma_m}{(1+k^2)^m} \\ \gamma_6 &= -\frac{7}{6}, \quad \gamma_5 = \frac{2}{9}, \quad \gamma_4 = \frac{11}{48}, \\ \gamma_3 &= \frac{13}{72}, \quad \gamma_2 = \frac{17}{1152}. \end{aligned} \right\} \quad (\text{A.10})$$

Collecting the terms that involve δv_k in (A.4), we find an extra contribution to the energy equal to half the cross term :

$$\sum_k \lambda_k \delta v_k = C\alpha^6 \quad (\text{A.11})$$

(A.11) is the first correction to the energy due to the *distortion* of the exciton wave function ϕ_{k0} when the density increases.

Using the same algebra (more and more tedious), we may calculate C :

$$C = \frac{-146.419\pi^2}{2.160}.$$

The total free energy (A.1) is thus

$$A\alpha^4 + (B+C)\alpha^6 - N\delta\mu \quad (\text{A.12})$$

which we must minimize with respect to α . Actually, in view of (A.5), we may replace α^2 by N in (A.12) with an accuracy $\sim N^4$. We then minimize with respect to N instead of α , which yields

$$\begin{aligned}\delta\mu &= 2AN + 3(B+C)N^2 \\ &= \frac{26\pi N}{3} - \frac{407\pi^2}{9}N^2\end{aligned}\quad (\text{A.13})$$

(A.13) extends our former result (25) to the next order — *in the limited framework of our mean field ansatz* (there are many other corrections of the same order).

The main interest of (A.13) is to provide a comparison with the simpler variational ansatz (30) used in section 3. In the dilute limit, we know that $\Omega = 1 - \eta$, where η is small. We thus write

$$\lambda_k = \frac{u_k v_k}{u_k^2 - v_k^2} = \frac{\zeta}{(1+k^2)(1+k^2-\eta)} \quad (\text{A.14})$$

(A.14) is supposed to interpolate between the known results in the dilute and dense limits. ζ and η are the variational parameters. When v_k is small, we may expand (A.14) as

$$\begin{aligned}v_k &= \lambda_k - \frac{3}{2}\lambda_k^3 + \dots = \frac{\zeta}{(1+k^2)^2} + \frac{\zeta\eta}{(1+k^2)^3} - \\ &\quad - \frac{3}{2} \frac{\zeta^3}{(1+k^2)^6} + \dots.\end{aligned}\quad (\text{A.15})$$

We carry (A.15) directly into (A.1) and (A.2), and we perform the integrals. We thus find

$$\begin{aligned}N &= \zeta^2 + \frac{5}{4}\eta\zeta^2 - \frac{99\pi}{2}\zeta^4 + \dots \\ F_0 &= \frac{\eta^2\zeta^2}{16} - 9\pi\eta\zeta^4 + \frac{37.953\pi^2}{80}\zeta^6 + \dots \\ F_1 &= \frac{13\pi}{3}\zeta^4 + 13\pi\eta\zeta^4 - \frac{30.249\pi^2}{40}\zeta^6 + \dots\end{aligned}\quad (\text{A.16})$$

$F_2 = \beta\alpha^6$ is the same as in (A.3). It is then easy to minimize $\langle H - \mu N \rangle$, first with respect to ζ and then with respect to η . We find

$$\begin{aligned}\eta &= \frac{82}{13}\delta\mu \\ \delta\mu &= 2AN + 3(B+C')N^2.\end{aligned}\quad (\text{A.17})$$

As compared with (A.13), the only difference is the replacement of C by

$$C' = -\frac{5701}{144}\pi^2.$$

The first order term $2AN$ is unaffected by our approximation (it does *not* depend on δv_k !). In the second order correction, the coefficient $C' \sim 0.58 C$ looks rather far from the exact value C . Indeed, when combined with the other term BN^2 , it gives the wrong sign for the net N^2 contribution to $\delta\mu$. It should be realized however that C results from near cancellation of various terms some 50 times larger : the fact that C' retains its small order of magnitude is by itself a fairly accurate result.

A more transparent way of assessing (A.15) is to write it in the form (A.3), by proper orthogonalization of the correction to ϕ_{k0} . We replace η by its expression (A.17), and we note that $\alpha = \zeta + 0(\zeta^3)$. We thus find

$$\delta v_k = (64\pi)^{3/2} \alpha^3 \sum_{m=2}^6 \frac{\bar{\gamma}_m}{(1+k^2)^m} \quad (\text{A.18})$$

$$\gamma_6 = -\frac{3}{2}, \quad \gamma_3 = \frac{41}{48}, \quad \gamma_2 = -\frac{113}{768}.$$

The approximate result (A.18) is plotted on figure 11, as well as the exact result (A.10). Our approximate ansatz (A.14) is seen to represent a rough — yet reasonable — approximation in the low density limit.

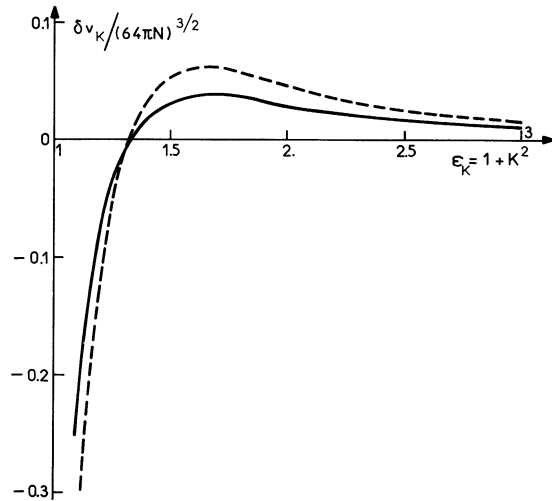


Fig. 11. — The first correction δv_k to the bare exciton internal wave function ϕ_{k0} , orthogonalized to ϕ_{k0} , as a function of $\epsilon_k = (1 + k^2)$, in the low density limit. The full line is the exact expression (A.10), the dotted line is the rough ansatz (A.18) used in section 3.

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