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MASTER

MONOGRAFIAS DE FÍSICA

VI

THE MANY BODY PROBLEM

C. N. YANG

Lectures at the Latin American School of Physics
June 27 - August 7, 1960

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RIO DE JANEIRO BRASIL

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by

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The Many Body Problem

§1. Generalities

a) The problem

We shall consider a system of a large number N of identical, spinless, non relativistic particles. For convenience set $\hbar = 1$ and $2m = 1$, where m is the mass of the particle. All quantities will be then expressed in units of $(\text{length})^P$, P being positive or negative; e.g. $|E| = \ell^{-2}$.

The Schroedinger equation to be considered is:

$$\left[\sum_{i=1}^{N} (-\nabla_i^2) + V\right] \psi = E\,\psi \tag{1.1}$$

where

$$V = \sum_{i>j} v\,(r_{ij}) \tag{1.2}$$

and the $v\,(r_{ij})$ are taken to be spherically symmetric for simplicity. Furthermore, we apply box normalization with periodic boundary conditions (different boundary conditions could be taken, but the present choice is simplest). Denote by Ω the volume of the box.

The following conditions are imposed on $v(r_{ij})$:

i) Short range; specifically $v = 0$ for $r > r_{max}$.

ii) It has a repulsive core. Evidence for this exists in both atomic and nuclear cases: forces in the helium molecule, nuclear potentials deduced from high energy nucleon-nucleon scattering experi-

ments. Furthermore the absence of a repulsive core would lead to a collapse situation. This can be seen as follows: if the potential is of the form shown in fig. 1.1, i.e. attractive at short distances, the particles tend to come together, since this lowers the energy. If we consider all particles confined to a small region of dimension d within the box Ω (Fig. 1.2), and take the corresponding wave function as a trial wave function to compute the ground state energy of the system, we have, for a <u>Bose system</u>:

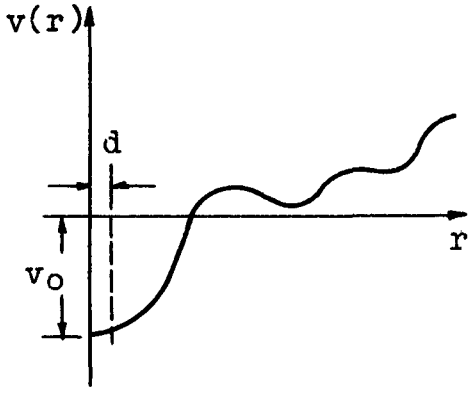


Fig. 1.1

$$< H > \sim - v_o \frac{N(N-1)}{2} + N\left(\frac{1}{d}\right)^2 \qquad (1.3)$$

as all particles can have the same $k \sim \frac{1}{d}$. Then, when N increases, the first term dominates and we get $E_o < -$ const. $\times N^2$. The system collapses, the density increasing indefinitely which is clearly an unphysical situation.

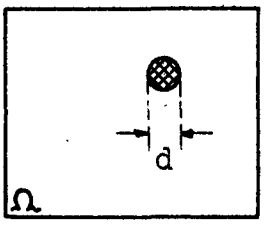


Fig. 1.2

For a <u>Fermi system</u>, not all particles can have the same wave length d. However let P be the maximum momentum of the Fermi sea. Choose as a trial wave function one representing independent particles in the small box of dimensions d; then

$$P^3 d^3 \sim N \quad \therefore \quad P \sim \frac{\sqrt[3]{N}}{d} \tag{1.4}$$

We get now:

$$< H > \sim - v_o \frac{N(N-1)}{2} + N \frac{\sqrt[3]{N^2}}{d^2} \tag{1.5}$$

For large N, the first term is again predominat, and the system collapses.

iii) The potential has a lower bound.

Example:

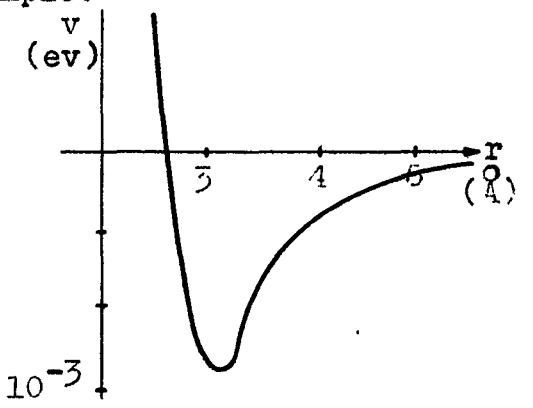


Fig. 1.3. Potential between two helium atoms. (London: "Superfluids" Vol. II).

b) <u>Ground state energy for a Bose system or a Boltzmann system</u>.

The wave function for a Bose system is symmetric under exchange of any two particles. Denote it by ψ_s. The wave function for a Boltmann system has arbitrary symmetry property. Denote it by ψ_{arb}.

<u>Theorem</u>: ψ_s (ground state) = ψ_{arb} (ground state)

Proof: Consider $\psi_{arb}^{g.s.}$ and interchange in it the coordinates of two particles; the resultant wave function is still a solution

of the Schroedinger equation with the same energy E_o, and so is the sum of the two wave functions. If we construct then the wave function

$$\Psi = \sum_P P\, \psi_{arb}^{g.s.} (r_1, \ldots, r_N)$$

where the sum extends to all possible permutations of two particles; Ψ satisfies the Schroedinger equation with eigenvalue E_o and is symmetric. As it does not vanish identically, ($\psi_{arb}^{g.s.}$ has no nodes and therefore is everywhere positive) we conclude that Ψ is the ground state wave function of the Bose system, q.e.d.

We are interested in the ground state energy for large N. First consider the case for a fixed N.

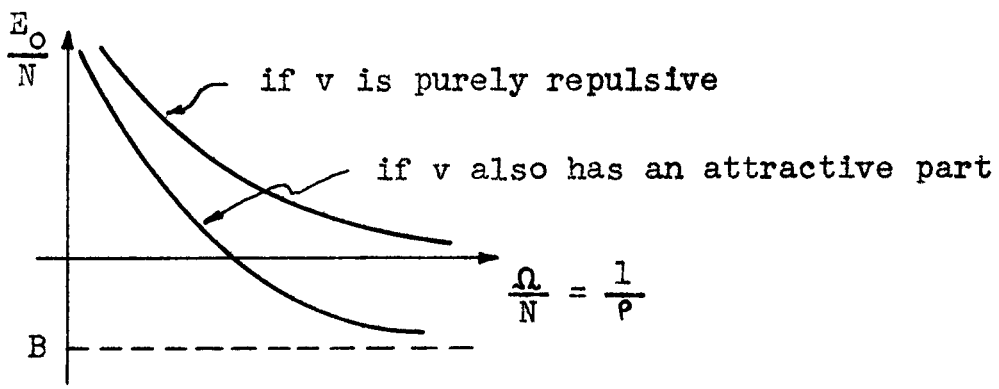


Fig. 1.4 - Ground state energy per particle vs. $(\text{density})^{-1}$.

Referring to Fig. 1.4, we can indeed prove that the curve is analytic, as it is a solution of Laplace's eq. with fixed boundary conditions and well behaved potentials. That the curve is monotonically decreasing is easily proved from the argument that an increase in volume

implies a reduction of constraints. That the energy approaches $+\infty$ for small Ω follows from the existence of the repulsive core.

As $\frac{1}{\rho} \longrightarrow +\infty$, the curve approaches $0+$ for a repulsive interaction (no attraction, therefore $E > 0$ always). Since the curve is monotonic and is bounded from below, $\lim_{\rho^{-1}\to\infty} \left(E/N\right)$ always exists. It is also easy to demonstrate that a lower bound B for E/N exists and B is independent of N. To see this we refer to Fig. 1.5. In the optimum arrangement of particles, i.e. corresponding to lowest

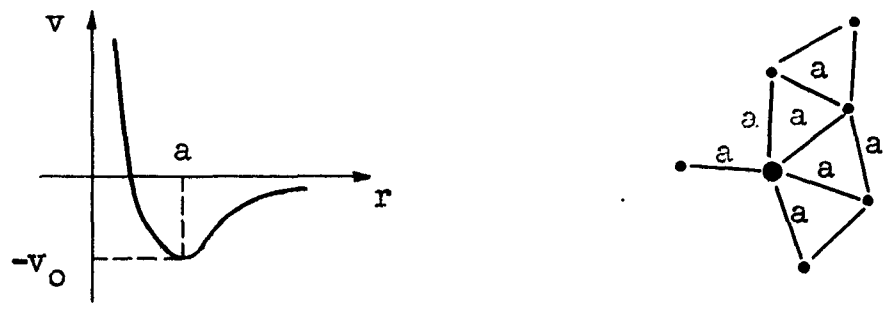


Fig. 1.5

energy, any given particle interacts only with a finite number $< \alpha$ of neighboring particles, and we have $E_o > -v_o \alpha N$. Therefore $\frac{E_o}{N} > -v_o \alpha$, independent of N.

Next consider the limit $N \longrightarrow \infty$, taken in such a way that ρ remains constant; we obtain the curves in Fig. 1.6. Three types, (i), (ii) and (iii), are possible. Again the curve is monotonic. It must concave upwards, and $\lim_{\substack{N\to\infty \\ \rho \text{ fixed}}} \left(E_o/N\right) = \infty$ at $\frac{\Omega}{N} = 0$. We distin-

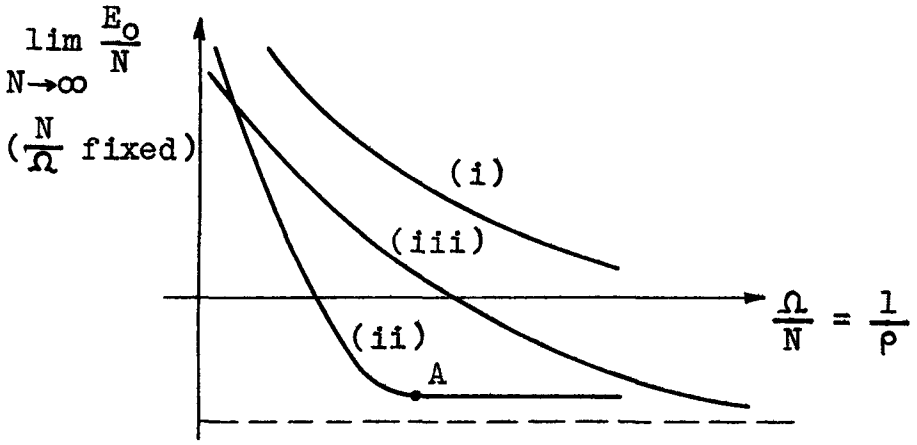


Fig. 1.6

guish three types of curves:

<u>type (i)</u>: $\lim \left(E_0/N\right) > 0$ always. Example: $v > 0$, the energy is always positive. The curve approaches zero because each individual curve (see Fig. 4) approaches zero uniformly in N.

<u>type (ii)</u>: the potential is partly attractive and allows bound states. As example, consider the case of nuclear matter. At $\frac{\Omega}{N} \sim 0$ the nuclear matter is compressed, the energy being therefore very high. As the volume increases, the density decreases (and so the energy) until the natural density of nuclear matter is reached, say at the point A. Beyond this point, we expect, physically, the nucleons to form a cluster which moves around as a single particle within the enlarged volume. The additional energy of the nucleus due to its motion is $\sim \frac{\hbar^2}{2Nm}\left(\frac{1}{L}\right)^2$. The energy per particle is $\frac{1}{N}\ \frac{\hbar^2}{2Nm}\left(\frac{1}{L}\right)^2$ which tends to zero as $N, L \to \infty$, that is, the displacement of the nucleus as a whole does not contribute to the energy per nucleon. The curve (ii)

is horizontal from the point A on. (Note: in any approximate theoretical calculation one usually gets a curve of the shape shown in Fig. 1.7. This is because one forces the particle to spread more than the natural density state, as if a negative pressure is applied).

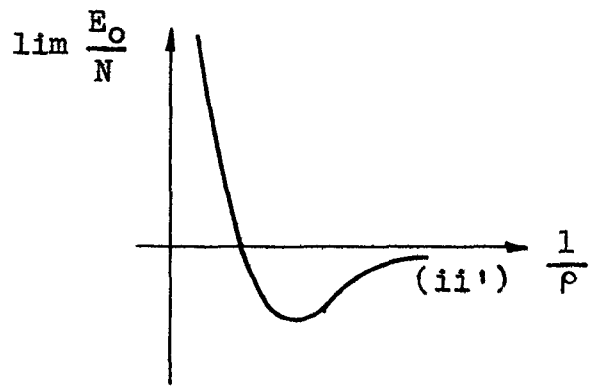


Fig. 1.7

<u>type (iii)</u>: the curve approaches smoothly a negative limit. It corresponds, for example, to a system in which two particles can be bound together, but not more.

In other words, for a system in which

$$0 > E(N=2,\Omega=\infty) = E(N=3,\Omega=\infty) = \frac{1}{2}E(N=4,\Omega=\infty) = \frac{1}{2}E(N=5,\Omega=\infty)$$
etc.

The two body clusters repel each other and this repulsion effect decreases as the volume, and therefore the distance between clusters, increases. That $\frac{E_o}{N}$ approaches a finite limit follows from the fact that now the energy is simply proportional to the number of two body clusters, i.e. $E_o \sim - v_o \frac{N}{2}$. Therefore $\frac{E_o}{N} \sim - \frac{v_o}{2}$.

c) <u>Ground state energy for a Fermi system</u>.

The discussion is similar to the Bose or Boltzmann case. Only the ground state energy of the Fermi system is higher than the ground

state energy of the Bose or Boltzmann case.

d) <u>Examples of a few questions not solved</u>.

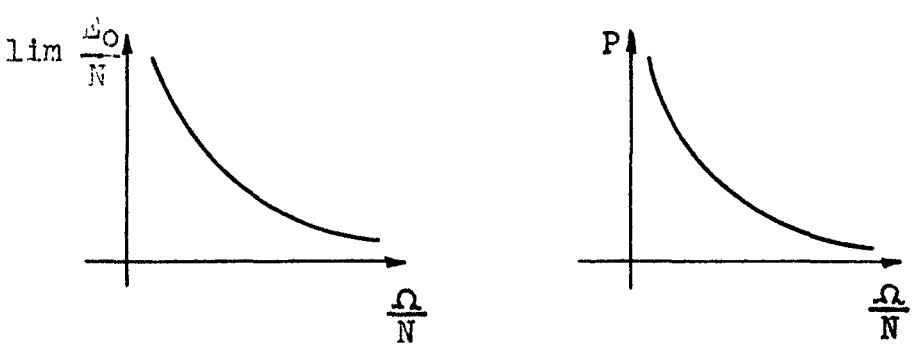
i) Does $\lim_{N\to\infty(\frac{\Omega}{N}\text{ fixed})}\left({}^{E_o}/_{N}\right)$ exist ? (It is believed that one can prove it exists).

ii) Is this limit independent of the boundary conditions ? (Tentative answer: yes).

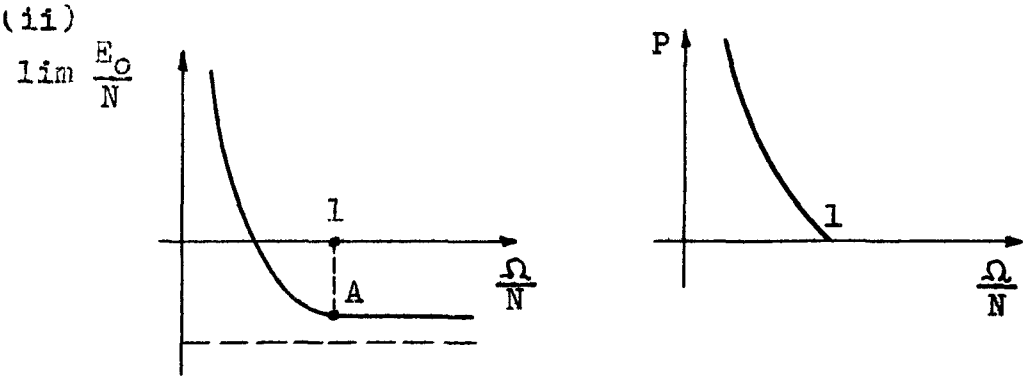
iii) Construction of an explicit example giving rise to the type (iii) curve in Fig. 6, section 1-b.

iv) The pressure of the system at zero temperature is by definition $P = -\left(\frac{\partial E_o}{\partial \Omega}\right)$. Consider the three curves in Fig. 1.6:

type (i)



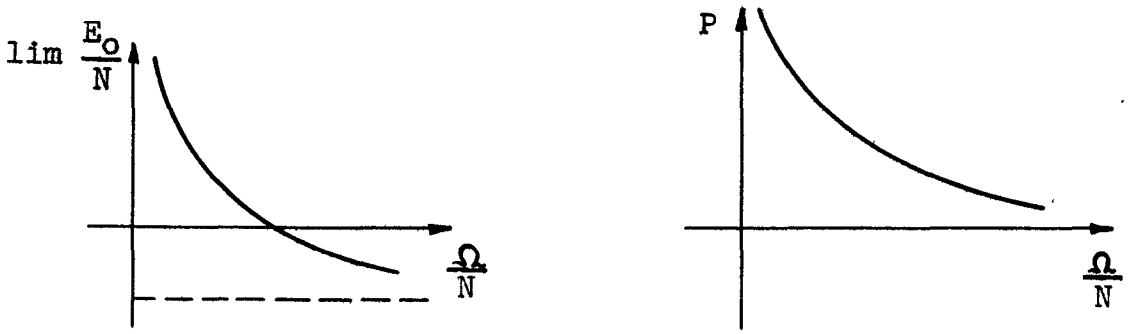
type (ii)



Can one prove that $P = 0$ as $\frac{\Omega}{N} = \left(\frac{\Omega}{N}\right)_A - 0$?

One can form a non rigorous proof by a variational argument near the point A.

type (iii)

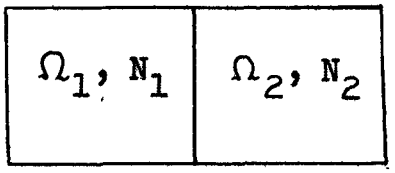


In this case p represents the pressure of the two body bound system.

v) For a hard sphere system, is the face-centered cubic packing the densest arrangement ? The answer is intuitively yes, but a mathematical proof is not yet known.

vi) Does the $\frac{E_o}{N}$ vs. $\frac{\Omega}{N}$ curve, for fixed N, concave upwards ? Does the lim $\frac{E_o}{N}$ vs. $\frac{\Omega}{N}$ curve, for $N \to \infty$, concave upwards ?

We can give an intuitive argument for answering yes to the second question. Referring to figure 1.8, construct a trial wave function which represents N_1 particles in Ω_1 and N_2 particles in Ω_2. Neglecting boundary effects at the intersurface of the



$$\Omega_1 + \Omega_2 = \Omega$$
$$N_1 + N_2 = N$$

Fig. 1.8

two boxes, a variational calculation yields:

$$E(N_1, \Omega_1) + E(N_2, \Omega_2) \geqslant E(N, \Omega)$$

or

$$\frac{N_1}{N}\left[\frac{E(N_1,\Omega_1)}{N_1}\right] + \frac{N_2}{N}\left[\frac{E(N_2,\Omega_2)}{N_2}\right] \geqslant \left[\frac{E(N,\Omega)}{N}\right] \quad (1.6)$$

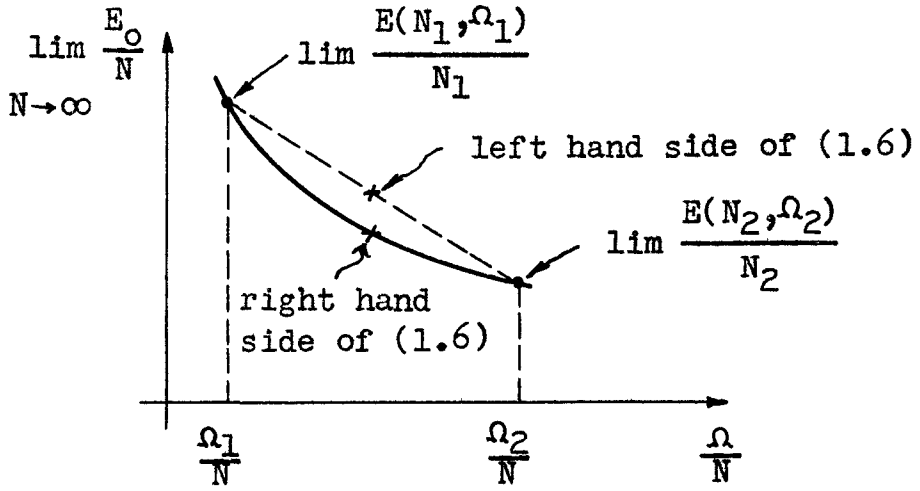


Fig. 1.9

It follows from eq. (1.6) that the point corresponding to the right hand side lies below the straight line joining the two points defined in the left hand side of eq. (1.6). The curve then concaves upwards.

e) Excited states

The definition of the excited states is not well formulated. In our scheme (box normalization), the excited states are boundary dependent, the density of states increasing as the volume of the box grows larger. The exact positions of the states is not of physical interest. Instead certain boundary independent quasi-stationary states are of physical importance.

The questions of the definition of the quasi stationary states, of their collision mean free path, lifetime and of the number of quantum numbers needed to characterize them, are not well settled. The problem is usually tackled in a way similar to the case of elementary particles: the actual Hamiltonian is divided conveniently into two parts, $H = Ho + H_{int}$, (as the strong and weak interaction parts in elementary particles), in such a way that Ho yields the ground state and the quasi stationary excited states of a quantum mechanical system, e.g. phonons and elementary particles, and H_{int} describes the residual (weak) interactions between the particles, which give the decay of the quasi stationary states.

f) Physical problems

We aim to obtain a qualitative understanding of the following questions:

i) Behaviour of He^4: λ transition at 2.2^o K, superfluidity, infinite heat conductivity below 2.2^o K, the two fluid problem (phenomenon of second sound).

ii) He^3: obeying Fermi instead of Bose statistics, it does not show the same phenomena as He^4.

iii) Nuclear matter: how to obtain the binding energy per nucleon from the interaction between nucleons.

iv) Superconductivity

We shall not discuss iv) at all.

Authors in this field: Schwinger, Martin, Brueckner, Bethe, Goldstone, Montroll, Van Hove, Watson, Bloch, de Dominicis, Luttinger, Klein, Ward, Galitzki, Beliaiev.

§2. Pseudopotentials for hard sphere interaction for two bodies.

(Phys. Rev. 105, 767 (1957))

a) Motivation

i) The hard sphere system constitutes a definite model in which we can estimate the accuracy of the approximations made. It has one obvious parameter, the diameter a of the hard sphere, in terms of which we obtain a series expansion of the energy.

ii) Physical reasons: a repulsive core exists in fact in the actual interactions.

iii) For a dilute system, which is the only system subject to relatively easy perturbation calculation, the important changes in the system brought about by the potentials is the change of wave function at large distances. This change is characterized by the phase shift, which for small energies, is in turn specified by the scattering length. The hard sphere potential is one in which the diameter a is precisely the scattering length.

b) The idea

It consists in replacing the interaction by suitable boundary conditions, and introducing a pseudopotential as an equivalent to the boundary conditions (Ref.: Fermi, Breit, Blatt and Weisskopf(*)).

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* E. Fermi, Ricerca Sci. 7, 13 (1936).
G. Breit, Phys. Rev. 71, 215 (1947).
J. M. Blatt and V. F. Weisskopf, Theoretical Nuclear Physics, John Wiley, New York, 1952, p. 74.

We shall treat first the two body problem.

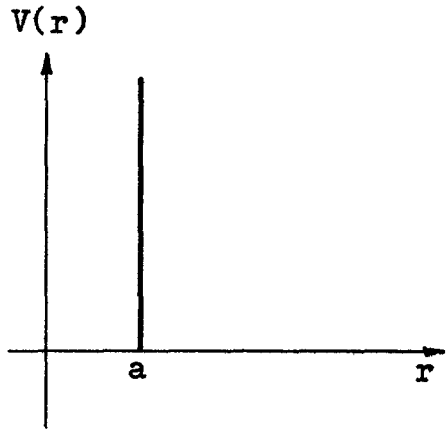


Fig. 2.1

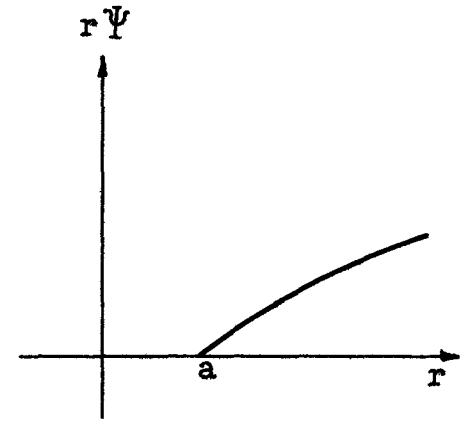


Fig. 2.2

For the potential of Fig. 2.1 the Schroedinger equation is, in relative coordinates:

$$(\nabla^2 + k^2)\ \psi(\vec{r}) = 0 \qquad r > a$$

$$\psi(\vec{r}) = 0 \qquad r \leq a \tag{2.1}$$

Let us consider for the moment only s waves. Expanding the wave function around the point a, we have

$$r\ \Psi \sim C(r - a)$$

or

$$\Psi \sim C\left(1 - \frac{a}{r}\right)$$

We extend this wave function up to the origin and look for the equation it satisfies:

$$\nabla^2 \Psi \sim - C\ a \nabla^2 \left(\frac{1}{r}\right) = 4\pi\ Ca\ \delta^3(r) \cong 4\pi\ a\ \delta^3(r)\ \Psi(0) \tag{2.2}$$

C is the value of Ψ for the unperturbed system.

One can not carry this argument to higher order, because one

obtains divergences due to the δ function interaction.

c) Formulation

Assume a hard sphere interaction only for s waves. Referring to fig. 2.3 we want to find a solution in the region limited by the sphere of radius a and any closed surface S. Ψ vanishes at both boundaries. The s wave satisfies:

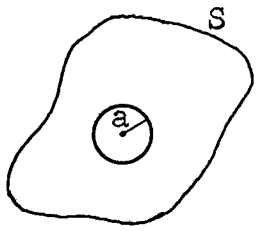


Fig. 2.3

$$(\nabla^2 + k^2)\Psi = 4\pi \frac{\tan ka}{k} \delta^3(r) \frac{\partial}{\partial r}(r\Psi) \tag{2.3}$$

where $k^2 = E$. This equation is equivalent to (2.2) for small k. We can prove it is an exact expression as follows: in the neighbourhood of the sphere, expanding Ψ, one can write

$$\Psi = \psi_s + \psi_P + \psi_d + \dots \quad ;$$

then $(\nabla^2 + k^2)\Psi = (\nabla^2 + k^2)\psi_s$ as the other terms vanish.

But

$$\psi_s = A \frac{\sin k(r-a)}{r} = A \frac{\sin kr}{r} \cos ka - A \frac{\cos kr}{r} \sin ka$$

Therefore

$$(\nabla^2 + k^2)\psi_s = A\, 4\pi\, \delta^3(r) \sin ka \tag{2.4}$$

On the other hand

$$4\pi \frac{\tan ka}{k} \delta^3(r) \frac{d}{dr}(r\Psi) = 4\pi \frac{\tan ka}{k} \delta^3(r) \frac{d}{dr}(r\,\psi_s) =$$

$$= A\, 4\pi \tan ka \cos ka\ \delta^3(r). \quad (2.5)$$

i.e. we obtain the same result as in (2.4).

d) Let us make a few remarks about this formulation:

(i) - Equation (2.3) is not in a most convenient form:

you may write it

$$k^2\Psi = \left[-\vec{\nabla}^2 + 4\pi \frac{\tan ka}{k} \delta(r) \frac{\partial}{\partial r} r \right] \Psi .$$

The operator k^2 is just the energy of the system: the laplacian is the kinetic energy, the pseudopotential is the potential energy, but this expression contains k^2 by itself. One way is to solve it explicitly, but, if we are interested in an expression of the problem in terms of a, we may write:

$$\frac{\tan ka}{k} = a \left[1 + \frac{1}{3} k^2 a^2 \right] + \ldots$$

the first term is independent of energy, the second is dependent but we can go back to the above expression of k^2. We can substitute the k^2 by the laplacian, up to higher order terms in a

$$\frac{\tan ka}{k} \sim a \left[1 - \frac{1}{3} a^2 \nabla^2 + \ldots \right]$$

One has additional terms in a^5. If we restrict ourselves to the two first terms there are no more k in the pseudopotential.

(ii) - The operator $\frac{\partial}{\partial r} r$ is not hermitian. One must be very careful about it - the operator has to be taken at the point r = 0.

If it operates on a function which is regular at the origin, then:

$$\frac{\partial}{\partial r} r \Psi \Big|_{r=0} = \Psi \Big|_{r=0}$$

which means that $\frac{\partial}{\partial r} r$ is just unity.

If the function is not regular, this is not true: for example, if $\Psi = \frac{1}{r}$, $\Psi \Big|_{r=0}$ is infinite, but if you put $\Psi = \frac{1}{r}$ in the left hand side, you have 0. So, $\frac{\partial}{\partial r} r \Psi \Big|_{r=0} \neq \Psi \Big|_{r=0}$ if the function is not regular at the point $r = 0$.

(iii) Higher harmonics. We follow the same procedure as for s waves; the details are discussed in the paper mentioned at the beginning of this section.

(iv) Let us mention an electrostatic analogue. This analogy is fundamental for the pseudopotential method.

Consider an electrostatic problem with a small conducting sphere at potential = 0. It is well known that we can replace the charges on the sphere by a single charge and a set of multipoles at the center of the sphere. If we sum up the actions of the multipoles, the potential produced outside the sphere is identical to the original potential. Ordinarily, we solve electrostatic problems this way. The analogy can be carried out now: the first term, the single charge, is just the s-wave of the scattering, the dipole is the p-wave, etc. If we want to see how to generalize the pseudopotential to the many body problem, the concept of equivalent multipole distribution will become very handy.

§3. Example of a perturbation calculation

Because of the fact that $\frac{\partial}{\partial r} r$ is a rather unfamiliar operator, we have to understand how it works, then we shall be able to apply it to more complicated problems. Let us take the very trivial problem of a wave function vanishing on the surface of two concentric spheres (figure 3.1).

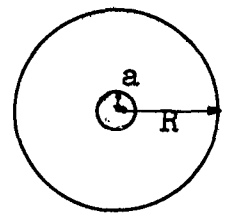


Fig. 3.1

We can write out the exact normalized solution

$$\Psi_n = \frac{1}{\sqrt{2\pi\,(R-a)}}\;\frac{\sin k_n(r-a)}{r} \qquad (3.1)$$

where

$$k_n = \frac{\pi n}{R-a}\quad,\quad n = 1, 2, 3 \ldots \qquad (3.2)$$

We want to expand this for small values of a:

$$\Psi_n = \psi_n^{\,o} + \psi_n^{\,1} + \ldots \qquad E_n = E_n^{\,o} + E_n^{\,1} + \ldots = k_n^{\,2} = \frac{\pi^2}{(R-a)^2}\,n^2$$

For example, from direct expansion we have

$$E_n^{\,o} = \frac{\pi^2 n^2}{R^2}\,,\quad E_n^{\,1} = \frac{\pi^2 n^2}{R^2}\,\frac{2a}{R}\,,\quad E_n^{\,2} = \frac{\pi^2 n^2}{R^2}\,3\left(\frac{a}{R}\right)^2 \qquad (3.3)$$

$$\psi_n^{\,o} = \frac{\sin\frac{\pi n r}{R}}{r}\;\frac{1}{\sqrt{2\pi R}} \qquad (3.4)$$

We know the exact solution and we can expand in terms of a. If we want to replace the boundary condition on the small sphere by a pseudopotential, can we make the perturbation calculation and derive the wave function and energy correction, and get the identical result ? Let us treat only up to order a^2:

$$E\Psi = \left[-\nabla^2 + 4\pi\, a\, \delta^3(\vec{r}) \frac{\partial}{\partial r} \right] \Psi \tag{3.5}$$

Let us write:

$$U = 4\pi\, a\, \delta(\vec{r}) \frac{\partial}{\partial r} r \tag{3.6}$$

In a perturbation expansion, the familiar matrix element is: $U_{mn} = \langle \psi_m^{\circ} | U | \psi_n^{\circ} \rangle$. This quantity is trivially calculable: ψ_n° is regular at the origin, so U is just a δ function

$$U_{mn} = 4\pi\, a\, \psi_m^{\circ}\, \psi_n^{\circ} \Big|_{r=0} = \frac{4\pi a}{2\pi R} \cdot \frac{\pi n}{R} \cdot \frac{\pi m}{R} = \frac{2a\pi^2}{R^3}\, mn \tag{3.7}$$

So we get the first order correction to the energy:

$$E_n^1 = \frac{2a\pi^2}{R^3}\, n^2$$

and this is the correct result obtained in eq. (3.3).

Let us calculate the second order energy. By a simple perturbation method:

$$\sum_{m \neq n} \frac{U_{nm}\, U_{mn}}{E_n^{\circ} - E_m^{\circ}} = \sum_{m \neq n} \frac{m^2\, n^2}{n^2 - m^2} \times \text{Cst.} \tag{3.8}$$

which is divergent: we get infinities. The reason for this infinity is an incorrect use of perturbation calculation. When one deri-

ves this formula one uses the hermiticity of the hamiltonian, which is not legitimate here. So the correct way is to proceed step by step:

$$\left|\psi_n^1\right\rangle = \sum_{m \neq n} \frac{U_{mn}}{E_n^o - E_m^o} \left|\psi_m^o\right\rangle \tag{3.9}$$

then we get the second order energy $E_n^2 = \langle \psi_n^o \mid U \mid \psi_n^1 \rangle$

$$E_n^2 = \langle \psi_n^o \mid U \mid \sum_{m \neq n} \frac{U_{mn}}{E_n^o - E_m^o} \psi_m^o \rangle \tag{3.10}$$

This formula is general. If you switch U with the summation, then you put out of the matrix element the constants and just have the expression (3.8). But you are not allowed to do it: U is acting on a sum which is not regular at the origin:

$$\sum_{m \neq n} \frac{U_{mn}}{E_n^o - E_m^o} \left|\psi_m^o\right\rangle = - \frac{2an}{r\,R\sqrt{2\pi R}} \sum_{m \neq n} \frac{m}{m^2 - n^2} \sin \frac{m\,\pi\,r}{R}$$

This Fourier sum has a kink at the point r = 0; it may be explicitly summed:

$$- \frac{2an}{r\,R\sqrt{2\pi R}} \frac{\pi}{2} \left[\left(\frac{\theta}{|\theta|} - \frac{\theta}{\pi} \right) \cos n\,\theta - \frac{1}{2} \frac{\sin n\,\theta}{\pi\,n} \right]$$

where $\theta = \dfrac{\pi r}{R}$

this is the same ψ_n^1 as obtained from direct expansion of the exact solution (3.1).

For $r = 0$, $\theta = 0$ but $\frac{\theta}{|\theta|} = 1$; ψ_n^1 behaves then like $\frac{1}{r}$.

Now if we use $E_n^2 = \langle \psi_n^o \mid U \mid \psi_n^1 \rangle$ we get the correct expression:

$$E_n^2 = 3 \frac{a^2}{R^2} \frac{\pi^2}{R^2} n^2 \qquad (3.10)$$

How the caclulation can be extend to higher orders: The pseudopotential is not exactly $U = 4 \pi a \delta(\vec{r}) \frac{\partial}{\partial r} r$. With the a^3 correction you get the right result in the next order.

We have seen that the existence of infinity come from the incorrect switching of the summation with U.

We shall do the same for the many body problem; we shall be able to eliminate the divergence and obtain the correct result.

§4. <u>Pseudopotential for the many body problem</u>.
(Phys. Rev. <u>105</u>, 767, (1957)).

For the many body problem, one is immediately led to write down the two body pseudopotentials:

$$V_{ps} = \sum_{i>j} 8 \pi a \delta^3(r_{ij}) \frac{\partial}{\partial r_{ij}} r_{ij} + \text{higher order}$$

terms.

The change of the factor 4 to 8 is because of the reduced mass: one has $\vec{\nabla}_1^2 + \vec{\nabla}_2^2 + \vec{\nabla}_3^2 + \ldots = \frac{1}{2} \nabla_R^2 + 2 \nabla_r^2 + \nabla_3^2 + \ldots$

where $\vec{R} = \frac{1}{2} (\vec{r}_1 + \vec{r}_2)$ and $\vec{r} = \vec{r}_1 - \vec{r}_2$. The kinetic energy

for the relative coordinate r is thus $2\nabla_r^2$. Hence the change from 4 to 8.

<u>Inaccuracies of V_{ps}:</u>

We must go back to the electrostatic picture: the problem is 3N-dimensional. The system is in a 3N-dimensional box, the function has to vanish or to be periodic on the surface of this box. Let us draw a "superline" $\vec{r}_1 = \vec{r}_2$ (see fig. 4.1); the boundary condition is $|\vec{r}_1 - \vec{r}_2| \leq a$, so we have to draw a small "cylinder" around this line: the dimension of the surface of this cylinder is 3N - 1, the boundary condition on this surface is $\Psi = 0$. Unfortunately, there are complications: There must be some point where the superline $\vec{r}_3 = \vec{r}_4$ intersects with the superline $\vec{r}_1 = \vec{r}_2$; in this region, the intersection of the two cylinders will be a complicated one.

We can make more higher order junctions: three cylinders, four ... The wave function of the system has to vanish on the surface of all these cylinders.

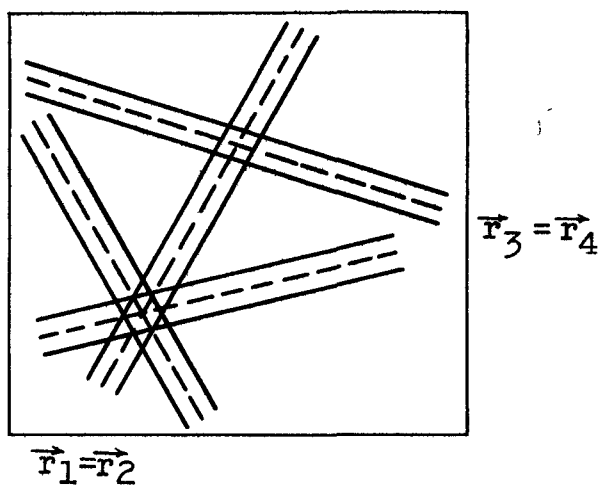


Fig. 4.1

Based on the electrostatic analogue, we might think of some charge distribution that gives rise to induced charges on the surface of the cylinder. If we use the concept

of multipole expansion, we replace the charges on the surface by charge and multipoles at the origin, that is on the axis of the cylinders. We have a pseudopotential distribution.

If we take the two body pseudopotentials, we can see that it does not properly take into account what is happening at the junctions. However the total surface area of the junction is small compared with the surface of the cylinders: we can take into account the junction of cylinders by terms in which products of several δ functions appear. For example, the junction of 2 cylinders may be written: $\delta(\vec{r}_1 - \vec{r}_2)\ \delta(\vec{r}_3 - \vec{r}_4)$. This term is of the order of a^4.

In the many body problem, nobody has taken into account these junctions properly. In the calculations below they can be neglected.

Solving the equation is easier if one uses the language of second quantization, because of the summations in the pseudopotential.

With a sum $\sum_{i>j} V_{ij}$, with a symmetrical expression of V_{ij}, you always get an expression:

$$V_{ps} = \tfrac{1}{2}\iint \Psi^*(\vec{r}_2)\ \Psi^*(\vec{r}_1)\ 8\pi a\, \delta^3(\vec{r}_1-\vec{r}_2)\ \frac{\partial}{\partial r_{12}}\, r_{12}\, \Psi(\vec{r}_1)\, \Psi(\vec{r}_2).$$

$$\cdot\, d\vec{r}_1\, d\vec{r}_2 \qquad (4.2)$$

where $\Psi(\vec{r})$ satisfies the commutation rules:

$$[\,\Psi(\vec{r}),\ \Psi(\vec{r}\,')\,]_{\pm} = 0\ , \quad [\,\Psi(\vec{r}),\ \overset{*}{\Psi}(\vec{r}\,')\,]_{\pm} = \delta^3\,(\vec{r}-\vec{r}\,'). \quad (4.3)$$

The number of particles is

$$N = \int \Psi^*(\vec{r}) \quad \psi(\vec{r}) \quad d\vec{r}$$

§5. <u>First order energy for a many body system</u>

This is easy because there are no divergences. Let us take periodic boundary conditions, and let us discuss energy correction only for the ground state of the system. Let us stay in the first quantization formulation for a Bose system. The wave function is

$$\Psi^o = \frac{1}{\sqrt{\Omega^N}} \tag{5.1}$$

and the first order ground state energy is

$$E^1_{gr} = \langle \Psi^o \mid V_{ps} \mid \Psi^o \rangle. \tag{5.2}$$

$\frac{\partial}{\partial r_{ij}} r_{ij}$ operating on Ψ^o - which is regular - gives one; we get $\delta(\vec{r})$ for each pair. The result is

$$E^1_{gr} = \frac{N(N-1)}{2} \times 8\pi a \frac{1}{\Omega} = 4\pi a \frac{N}{\Omega}(N-1). \tag{5.3}$$

If N is very large, the ground state energy is just $4\pi a\rho$, where $\rho = N/\Omega$ is the density.

We shall now do the energy calculation in the second quantization formalism. The pseudopotential is defined by eq. (4.2). This has the complication of the operator $\frac{\partial}{\partial r} r$. We stated before that for a function regular at the origin we can replace it by unity. We

shall then define the pseudopotential

$$V'_{ps} = 4\pi a \int \Psi^*(1)\, \Psi^*(2) \quad \delta(\vec{1}-\vec{2})\, \Psi(2)\, \Psi(1) \quad d\vec{1} \quad d\vec{2} \qquad (5.4)$$

We shall work with this operator until we get into difficulties, and then look back at the right expression. The advantage of V'_{ps} is that it has a much simpler form.

Let us consider a periodic box. The simplest way to work in the second quantization formalism is to expand into plane waves:

$$\Psi(\vec{r}) = \sum_k \frac{1}{\sqrt{\Omega}} \quad e^{i\vec{k}\cdot\vec{r}} \quad a_{\vec{k}} \quad ; \qquad (5.5)$$

k is a simple cubic lattice of points: $k = \frac{2\pi}{L} \times$ integer; the $a_{\vec{k}}$ are amplitudes which are quantized quantities. The commutation rules for them can be obtained from those for Ψ, eq. (4.3):

$$\begin{aligned} [\, a_{\vec{k}} \,,\, a_{\vec{k}'} \,]_{\pm} &= 0 \\ [\, a_{\vec{k}} \,,\, a^*_{\vec{k}} \,]_{\pm} &= \delta_{\vec{k}\,\vec{k}'} \quad . \end{aligned} \qquad (5.6)$$

If we substitute the development for Ψ into V'_{ps}, we have:

$$V'_{ps} = \frac{4\pi a}{\Omega^2} \sum_{\vec{i}\vec{j}\vec{k}\vec{\ell}} a^*_{\vec{i}}\, a^*_{\vec{j}}\, a_{\vec{k}}\, a_{\vec{\ell}} \quad e^{i(-\vec{i}\cdot\vec{r}_1 - \vec{j}\cdot\vec{r}_2 + \vec{k}\cdot\vec{r}_2 + \vec{\ell}\cdot\vec{r}_1)} \delta(\vec{r}_1 - \vec{r}_2)\, d\vec{r}_1\, d\vec{r}_2$$

The double integral is a trivial one; it vanishes unless $\vec{i}+\vec{j}-\vec{k}-\vec{\ell} = 0$, in which case its value is Ω. The result is then

$$V'_{ps} = \frac{4\pi a}{\Omega} \sum_{ijk\ell} a^*_i\, a^*_j\, a_k\, a_\ell \quad \delta^3(i + j - k - \ell) \qquad (5.7)$$

where the δ is now a discrete one. We have suppressed the arrows in the momenta for simplicity; this convention will be used from now on.

The meaning of expression (5.7) is clear: it represents the scattering of two particles from $\vec{k}\,\vec{\ell}$ momentum state to $\vec{i}\,\vec{j}$, with conservation of momentum, summed over all possibilities of value and direction of momentum.

<u>Energy for a Bose system</u>

We label an arbitrary state by $|n\rangle$, where n represents the occupation numbers of the various momentum states: $n \equiv n_o\, n_1\, n_2 \ldots$ Let us calculate the diagonal matrix element $\langle n|V'_{ps}|n\rangle$. Consider any term of V'_{ps}; unless $\vec{k}$ and $\vec{\ell}$ are respectively identical to $\vec{i}$ and $\vec{j}$ we get zero. Then we are left with two cases:

a) $\vec{k} = \vec{\ell} = \vec{i} = \vec{j}$.

The operator a_k when applied on the state $|n\rangle$ gives a factor $\sqrt{n_k}$.

$$\sum_k \langle n|\, a_k^* \; a_k^* \, a_k \, a_k \,|\, n\rangle = \sum_k n_k\,(n_k - 1)$$

b) $\vec{i} \neq \vec{j}$

The scattering is $\vec{i}\vec{j} \rightarrow \vec{k}\,\vec{\ell}$ or $\vec{i}\vec{j} \rightarrow \vec{\ell}\,\vec{k}$. One term is of the form $a_k^*\, a_\ell^*\, a_k\, a_\ell$; the other has $a_\ell\, a_k$ but gives the same contribution $n_k\, n_\ell$.

The total contribution is

$$\langle n\ |V'_{ps}|\ n\rangle = \frac{4\pi a}{\Omega}\ \left[\sum_{K} n_k(n_k-1) + 2\sum_{\substack{K,K' \\ k\neq k'}} n_k\ n_{k'}\right] \tag{5.8}$$

We can write it

$$\langle n\ |V'_{ps}|\ n\rangle = \frac{4\pi a}{\Omega}\ \left[\sum_{K} n_k^2 - N + 2\ (\sum_{K} n_k)^2 - 2\ \sum_{K} n_k^2\right]$$

or finally

$$\langle n\ |V'_{ps}|\ n\rangle = \frac{4\pi a}{\Omega}\ \left[\ 2\ N^2 - N - \sum_{K} n_k^2\ \right] \tag{5.9}$$

In the case of the ground state $n_k = 0$, $k \neq 0$ and $n_o = N$. We get from eq. (5.9):

$$E^{(1)}_{g.s.} = \frac{4\pi a}{\Omega}\ (N^2 - N) \tag{5.10}$$

which is the expression (5.3) we got by the first quantization calculation.

When N is large, $E^{(1)}_{g.s.} \sim \frac{4\pi a}{\Omega}\ N^2$, i.e. the energy is proportional to $N\rho$.

<u>Discussion</u>: The expression (5.10) was in essence obtained by Lenz and Heitler in 1929 for the particular case of the ground state. They considered a big box in which particles are scattering on each other. Let us suppose that all the particles are fixed scatterers and one is going in: it has a scattered s wave on each scatterer, the waves superpose to give a wave travelling through the medium: the change in the wave number gives us a sort of index of refraction. The change in energy of the particle is known to be proportional to the density, for a medium of low density. We obtain the above depend-

ence on the density. A defect in such an argument is that the scattering centers are considered as fixed: it cannot be easily refined.

The third term of the expression (5.9) is a pure quantum mechanical term, due to Bose statistics. If we want to go to low energy states, we want to make the sum $\sum n_k^2$ as large as possible; the best is to put all the particles in the same momentum state; that is Bose - Einstein condensation: the particles tend to condense into one momentum state.

We can ask the question: which is the energy of the first excited state above the ground state ?

$$\Delta\langle n|V_{ps}|n\rangle = -\frac{4\pi a}{\Omega}\left[((N-1)^2+1) - N^2\right] = -\frac{4\pi a}{\Omega}(-2N+2)$$

which, for very large N is $\frac{4\pi a}{\Omega} \times 2N = 8\pi a\rho$.

The excited state has a finite energy difference from the ground state. The difference is independent of the size of the box when density is fixed. This is completely different from the excitation of a free particle: the kinetic energy difference $(\frac{1}{L})^2$ goes to zero as the box gets larger.

In the many particle case, we get an energy gap between the ground state and the first excited state, which is not the case in the free particle problem. However a more elaborated calculation does not yield an energy gap, as we shall see later on.

<u>Energy for a Fermi system</u>

The procedure is exactly the same as in the Bose case.

Let us be a little more general and include the spin. Every particle will be labelled by its momentum and a parameter S, which may take $2J + 1$ values: $-J, -J+1 \ldots J$. If there are two of these S, spin and isotopic spin, we can combine the two together. Thus S gives $J = \frac{1}{2}$ for protons alone, $J = 3/2$ for neutrons and protons. S gives the total degree of internal freedom.

It is well known that, when the potential is independent of spin, we get exactly the same expression as in the spinless case, the spins are not switched.

$$V'_{ps} = \frac{4\pi a}{\Omega} \sum_{\substack{k_1 k_2 k_3 k_4 \\ s_1 s_2 s_3 s_4}} a^*_{k_1 s_1} a^*_{k_2 s_2} a_{k_3 s_3} a_{k_4 s_4} \delta^3(k_1+k_2-k_3-k_4) \delta_{s_1 s_4} \delta_{s_2 s_3}$$

$$= \frac{4\pi a}{\Omega} \sum_{\substack{k_1 k_2 k_3 k_4 \\ s_1 s_2}} a^*_{k_1 s_1} a^*_{k_2 s_2} a_{k_3 s_2} a_{k_4 s_1} \delta^3(k_1+k_2-k_3-k_4)$$

$$= \frac{4\pi a}{\Omega} \sum_{\substack{k_1 k_2 k_3 k_4 \\ s_1 \neq s_2}} a^*_{k_1 s_1} a^*_{k_2 s_2} a_{k_3 s_2} a_{k_4 s_1} \delta^3(k_1+k_2-k_3-k_4) \qquad (5.11)$$

the terms $s_1 = s_2$ vanish because $a_{k_3 s_1} a_{k_4 s_1} + a_{k_4 s_1} a_{k_3 s_1} = 0$.

In other words only for identical spins there can be no s-state interaction between Fermions.

The diagonal element of V'_{ps} is easy to compute:

$$\langle n_{ks} | V'_{ps} | n_{ks} \rangle = \frac{4\pi a}{\Omega} \sum_{\substack{k_1 k_2 \\ s_1 s_2}} \underset{s_1 \neq s_2}{n_{k_1 s_1} n_{k_2 s_2}} \qquad (5.12)$$

this expression is equal to:

$$\frac{4\pi a}{\Omega}\left[\sum_{\substack{k_1k_2\\ s_1s_2}} n_{k_1s_1}\, n_{k_2s_2} - \sum_{s_1}\sum_{k_1k_2} n_{k_1s_1}\, n_{k_2s_1}\right]$$

The first term is the product of two sums $\sum_{k\,s} n_{ks} = N$. In the second term there are two independent summations: $\sum_s (\sum_k n_{ks})^2$

Thus

$$\langle n|V'_{ps}|n\rangle = \frac{4\pi a}{\Omega}\left[N^2 - \sum_s (\text{total number of particles with spin } S)^2\right]$$

In the ground state, all possible states S are equally occupied. There are $\frac{N}{2J+1}$ particles for a fixed spin S.

Then

$$\sum_{s_1}\sum_{k_1k_2} n_{k_1s_1}\, n_{k_2s_2} = \sum_{s_1}\left(\frac{N}{2J+1}\right)^2 = \left(\frac{N}{2J+1}\right)^2 (2J+1)$$

For the ground state:

$$\langle \text{gr.s.}|\, V'_{ps}\, |\,\text{gr.s.}\rangle = 8\pi a\rho\, N\, \frac{J}{2J+1} \qquad (5.13)$$

Comparing with the Bose expression, we must exclude the pair of particles having the same spin state. There are N particles in the ground state and 2J + 1 possible spin states. We must have $(N - \frac{N}{2J+1})$ particles that may interact with one particle:

$$E^1_{gs} = 4\pi a\rho\, N\left(1 - \frac{1}{2J+1}\right) \qquad (5.14)$$

§6. Higher order energies (Phys. Rev. 105, 767 (1957))

One can calculate the higher order terms. When we meet divergences the method to get rid of them is exactly the same as the two body problem. The procedure is very simple: we use straightforward perturbation until divergences are met. Let us write down the results:

Fermi system

If P_F is the maximum Fermi momentum:

$$P_F^3 = \frac{6\pi^2\rho}{2J+1} \; ; \; \rho = \frac{N}{\Omega}$$

$$\frac{E_g}{2} = \frac{3}{5} P_F^2 + 8\pi a\rho \frac{J}{2J+1} \left[1 + 6\,(11 - 2\ln 2) \frac{P_F a}{35\pi} + 0\,(P_F^2 a^2) \right]$$

The calculation of the terms is in principle very simple but a little bit involved. We have to be careful about the question of the switching of the pseudopotential with the sums.

Let us pay attemtion to the fact that each term gives a finite expression in the case of fixed ρ and a, as Ω and N go to infinity.

Bose system

$$\frac{E_g}{N-1} = 4\pi a\rho \left[1 + (2{,}37) \frac{\xi}{L} + \left(\frac{a}{L}\right)^2 \left[(2{,}37)^2 + \frac{\xi}{\pi^2} (2N-5) \right] + \ldots \right]$$

2,37 is the Madelung constant related to a lattice of positive point

charges with a negative constant charge distribution, $L^3 = \Omega$ and

$$\xi = \sum_{\substack{\ell,m,n=-\infty \\ \ell,m,n\neq 0}}^{+\infty} \frac{1}{(\ell^2+m^2+n^2)^2}$$

This sum can be shown to be convergent. In the Fermi case, the parameter Ω is all absorbed in ρ or P_F. It is not the same for Bose system. One is very interested in systems where ρ is fixed, and Ω, N go to infinity. We expect the calculated energy to be finite:

$\frac{a}{L}$, $(\frac{a}{L})^2$ approach zero; but N goes to infinity like L^3 and the term $N(\frac{a}{L})^2$ is infinite like L. For a fixed ρ, we cannot get a larger box without a smaller a, otherwise we get divergences immediately. For a fixed N and a fixed Ω, a has a very small region of validity.

It can only be applied to cases in which we are considering a finite number of particles, but a very large box; e.g. in the virial expansion, one is expanding in power of ρ, that means that we are always dealing with systems at $\rho = 0$, and getting derivation of various physical quantities at zero density. Virial calculation has been successfully made for the hard sphere problem.

§7. Energy for a Bose Einstein system at finite ρ

(Phys. Rev. 106, 1135 (1957))

We have met two kind of divergences: one is the infinite potential of the hard sphere problem; we must be careful about the

expansion and the incorrect use of the pseudopotential. The other is that the number of pairs of interacting particles increases like N^2 and we need only an increase of the order of N; for example, in the term $(\frac{a}{L})^2$ the trouble is that the coefficient is $(2N - 1)$.

How can we get rid of these difficulties ?

We are going to rearrange the sum in the energy and get finite results. There is no rigorous justification of it, since, if a series is divergent, there is always a way to rearrange it to get any finite result; but the rearrangement is a quite natural one and can be obtained by several different ways.

We have a hamiltonian

$$H = T + V_{ps} \tag{7.1}$$

where the kinetic energy T is given by

$$T = \sum_k k^2 \; a_k^* \; a_k \tag{7.2}$$

and the pseudopotential V_{ps} is given by eq. (4.2).

We shall deal first with

$$H' = T + V'_{ps} \tag{7.3}$$

until we meet some infinity.

$$V'_{ps} = \frac{4\pi a}{\Omega} \sum_{k_1 k_2 k_3 k_4} a_{k_1}^* \; a_{k_2}^* \; a_{k_3} \; a_{k_4} \quad \delta(\vec{k}_1 + \vec{k}_2 - \vec{k}_3 - \vec{k}_4)$$

The diagonal matrix elements of this operator are, as given by eq. (5.9)

$$\langle n \mid V'_{ps} \mid n \rangle = \frac{4\pi a}{\Omega} \left(2N^2 - N - \Sigma\, n_u^{\,2}\right) \tag{7.4}$$

For the ground state:

$$E_{g.s.} = \frac{4\pi a}{\Omega} \left(N^2 - N\right) \tag{7.5}$$

The essential of the physical idea we are going to use is the following: let us consider a state which is near the ground state; the occupation distribution in such a state is such that most of the particles are still in the ground state. If we start from the ground state, by an off-diagonal matrix element, we can only diminish the number of particles in the ground state by 2, and then again by 2; no matter how many times we excite through an off-diagonal matrix element of the interaction, we still have essentially the same occupation number of the ground state, since N is very large. Thus we are going to deal only with states such that the occupation number of the ground state is $n_o \sim N$ and the occupation number of the other states is $n_k \sim$ a finite number. We summarize this by

$$\begin{aligned} \frac{n_o}{N} &= 1 + 0\left(\frac{1}{N}\right) \\ \frac{n_k}{N} &= 0\left(\frac{1}{N}\right) \end{aligned} \tag{7.6}$$

This is not a mathematical statement, but it is clear what it

means physically.

Let us see what is the <u>diagonal matrix element</u> for these states:

$$\langle n \mid V'_{ps} \mid n \rangle - \frac{4\pi a}{\Omega}(N^2 - N) = \frac{4\pi a}{\Omega}\left(-\sum_k n_k^2 + N^2\right) \tag{7.7}$$

$$= \frac{4\pi a}{\Omega}\left(-\sum_k{}' n_k^2 - n_o^2 + N^2\right)$$

where the prime in the summation indicates that the term k = 0 is to be excluded. n_o is slightly different from N; for the squares we have to be careful

$$N^2 - (N - \Sigma' n_k)^2 = 2N \ \Sigma' n_k - (\Sigma' n_k)^2$$

$$\langle n|V'_{ps}|n\rangle - \frac{4\pi a}{\Omega}(N^2 - N) = \frac{4\pi a}{\Omega}\left[-\sum_k n_k^2 + 2N\,\Sigma' n_k - (\Sigma' n_k)^2\right] \tag{7.8}$$

These are drastically different orders of magnitude: $2\,N\,\Sigma' n_k$ is the dominating term. The others are neglegible. Thus

$$\langle n \mid V'_{ps} \mid n \rangle \cong 4\,\pi\,a\,\rho\,(N - 1) + 8\,\pi\,a\,\rho\,\Sigma' n_k \tag{7.9}$$

Let us look at the <u>off-diagonal matrix elements</u> of the potential

$$V'_{ps} = \frac{4\pi a}{\Omega} \sum_{1234} a_1^* \ a_2^* \ a_3 \ a_4 \ \delta^3(1 + 2 - 3 - 4)$$

Let us remember that each term in the sum give us a contribution to a process which can be described as the scattering from momentum

states $\vec{k}_1 \vec{k}_2$ to $\vec{k}_3 \vec{k}_4$. Each a_k operator gives us a factor $\sqrt{n_k}$. We are dealing with states which have the characteristics summarized in (7.6); their matrix elements are going to have drastically different order of magnitude.

What are the largest off-diagonal matrix elements, as far as the order of N is concerned ? There are several classes of elements:

(i) the four momenta involved are zero: this gives only diagonal matrix elements.

(ii) the state $k_1 = k_2 = k_3 = 0$ and $k_4 \neq 0$ is not possible, because of momentum conservation. This is a very important statement: with a boundary condition that Ψ vanishes on the wall, we get exactly the same procedure; the fact that the walls can reflect is equivalent to non conservation of momentum; at this last point we get into trouble, the calculations become much more complicated. This may be understood easily: the distribution of the density in the box with perfectly reflecting walls is rather unphysical, since it has a maximum at the center of the box. A periodic box gives us a constant density all over the box; the physical situation is a constant density inside the box, with a rapidly decreasing density on the walls. The difficulties in the case of reflecting walls mean that we are taking a wrong way to calculate the features of the system. For an easy calculation the unperturbed system must be very close to the real system. With a periodic box, we have a greater chance of success.

(iii) Two momenta are zero: it must be the pair $\vec{k}_3 \vec{k}_4$ or $\vec{k}_1 \vec{k}_2$

otherwise it gives only diagonal matrix elements. There are two kinds of largest off-diagonal matrix elements:

$$\vec{k}_1 = \vec{k} \qquad \vec{k}_2 = -\vec{k} \qquad \vec{k}_3 = \vec{k}_4 = 0$$

and

$$\vec{k}_1 = \vec{k}_2 = 0 \qquad \vec{k}_3 = +\vec{k} \qquad \vec{k}_4 = -\vec{k}$$

As far as N is concerned, the magnitude of these elements is easily calculated:

$$\frac{4\pi a}{\Omega} n_0 \sim \frac{4\pi a}{\Omega} N \sim 4 \pi a \rho$$

these elements are finite when N, Ω go to infinity.

(iv) There are smaller off-diagonal matrix elements:

$$k_4 = 0, \qquad k_3 \neq 0$$

$$\vec{k}_3 = -\vec{k}_2 + \vec{k}_1$$

it is obvious that they are smaller by a factor $\frac{1}{\sqrt{N}}$.

(v) no momentum is zero. They are smaller by the factor $\frac{1}{\sqrt{N}}$. The elements of classes (iv) and (v) are infinitely smaller than the largest ones (class (iii)) but there are infinitely more of them e.g. there are many more elements of the fourth kind than of the third.

We shall proceed to do a calculation by first neglecting elements of classes (iv) and (v) and then show that they can be

included perturbationwise to give corrections of the order $\sqrt{\rho a^3}$.

We remark that in recent years in the theory of superconductivity people have, in a very similar manner, neglected certain off-diagonal elements and kept some others. However, there has been no justification whatsoever of this procedure since no one has successfully estimated the error committed in making the approximation. Worse still, the magnitude of the off-diagonal elements kept is the same as those neglected, while there are infinitely more neglected ones than kept ones.

Let us now calculate <u>the energy of a Bose system</u>.

The off-diagonal matrix elements of V'_{ps} can be replaced by those of V''_{ps} defined by

$$\left(V'_{ps}\right)_{\text{off.d.}} = \left(V''_{ps}\right)_{\text{off. d.}}$$

$$V''_{ps} = \frac{4\pi a}{\Omega} \sum_k{}' a_{\vec{k}}^* \, a_{-\vec{k}}^* \, N + \frac{4\pi a}{\Omega} \sum_k{}' a_{\vec{k}} \, a_{-\vec{k}} \, N \qquad (7.10)$$

The factors $a_o \, a_o$ or $a_o^* \, a_o^*$ give $n_o \sim N$. This hamiltonian clearly gives us the off-diagonal matrix elements of the kind (iii). When we have accepted the approximation, we have a very simple calculation. The diagonal matrix elements are $8 \pi a \rho \sum_k{}' a_k^* \, a_k$. We must not forget the kinetic energy and the ground state energy:

$$H'' = \Sigma' k^2 a_k^* \, a_k + 8 \pi a \rho \, \Sigma' a_k^* \, a_k + 4 \pi a \rho (N-1) + 4 \pi a \rho \times$$
$$\times \Sigma'(a_k^* \, a_{-k}^* + a_k \, a_{-k}) \qquad (7.11)$$

k summation ranges over all $\vec{k} \neq 0$. This hamiltonian is quadratic in the operator a; it is obvious that by a correct transformation, we can completely diagonalize it:

Let us replace $\sum_k'$ by $2 \sum_{\frac{1}{2}k}$ where k ranges over the half space.

$$H'' = 4\pi a\rho(N-1) + \sum_{\frac{1}{2}k}'(a_k^* a_k + a_{-k}^* a_{-k})(k^2+8\pi a\rho) + \sum_{\frac{1}{2}k} 8\pi a\rho(a_k^* a_{-k}^* + a_k a_{-k})$$

Let us define the operators:

$$b_k = \alpha a_k + \beta a_{-k}^* \qquad b_{-k} = \alpha a_{-k} + \beta a_k^* \qquad (7.12)$$

the commutation rules are:

$$[b_k, b_{-k}] = 0 \qquad [b_k, b_{-k}^*] = 0 \qquad [b_k^*, b_{-k}^*] = 0 \qquad (7.13)$$

$$[b_k, b_k^*] = \alpha^2[a_k, a_k^*] - \beta^2[a_{-k}^*, a_{-k}^*] = \alpha^2 - \beta^2 .$$

We choose α, β such that this is 1. Then the b operators follow the same rules as the a: they are creation and annihilation operators.

Let us substitute a in terms of b into H. Let us write the transformation inverse to (7.12).

$$\alpha b_k - \beta b_{-k}^* = a_k$$

$$\alpha b_{-k} - \beta b_k^* = a_{-k} \tag{7.14}$$

The undesirable (non diagonal) terms are:

$$(k^2 + 8\pi a\rho)\left[-2\alpha\beta b_{-k}b_k - 2\alpha\beta b_{-k}^* b_k^*\right] + 8\pi a\rho(\alpha^2+\beta^2)(b_k b_{-k} + b_k^* b_{-k}^*)$$

If we put

$$(k^2 + 8\pi a\rho)\, 2\alpha\beta = 8\pi a\rho(\alpha^2+\beta^2) \tag{7.14}$$

Then the crossed terms vanish identically. This may be accomplished choosing

$$\beta = \sinh\theta, \alpha = \cosh\theta, \tanh 2\theta = \frac{8\pi a\rho}{k^2+8\pi a\rho} . \tag{7.14}$$

It is seen that there is always a solution for α and β .

Denoting

$$k_o^2 = 8\pi a\rho. \tag{7.15}$$

the diagonal terms of the hamiltonian then give

$$H'' = 4\pi a\rho(N-1) + \sum_{\text{all } k \neq 0}{}' (k^2 + k_o^2)[\alpha^2 b_k^* b_k + \beta^2 b_k b_k^*] +$$

$$+ \sum_{\text{all } k \neq 0}{}' k_o^2 \left[-\alpha\beta(b_k b_k^* + b_k^* b_k\right] .$$

Using the commutation rules for the b's and expressing α and β as functions of θ (eq. (7.14)),

$$H'' = 4\pi a\rho(N-1) + \sum_k{}' \left[(k^2 + k_o^2)\cosh 2\theta - k_o^2 \sinh 2\theta\right] b_k^* b_k +$$

$$+ \sum_k{}' \left[(k^2 + k_o^2)\sinh^2\theta - k_o^2 \tfrac{1}{2}\sinh 2\theta\right]$$

Using (7.14) and (7.15) we get finally

$$H'' = 4\pi a\rho(N-1) + \sum_k{}' \sqrt{k^4 + 2k_o^2 k^2}\, b_k^* b_k - \tfrac{1}{2}\sum_k{}' \left[k^2 + k_o^2 - \sqrt{k^4 + 2k^2k^2}\right] \tag{7.16}$$

The second term, because of the factor $b_k^* b_k$, represents the excitation energies. The other two give the ground state energy.

This expression diverges. To see this, we can write for large k:

$$k^2 + k_o^2 - \sqrt{k^4 + 2k_o^2k^2} = k^2 + k_o^2 - k^2\sqrt{1 - \frac{2k_o^2}{k^2}} \simeq k^2 + k_o^2 - k^2\left(1 + \frac{k_o^2}{k^2} - \frac{k_o^2}{2k^4} + \ldots\right)$$

$$\simeq \frac{k_o^4}{2k^2}$$

Then

$$\sum_k{}' \frac{k_o^4}{2k^2} \longrightarrow \text{const.} \int \frac{1}{k^2}\, d\vec{k} = \text{const.} \int_0^\infty dk = \infty$$

As in the two body case treated earlier, this divergence arises from using H'', where $\frac{\partial}{\partial r} r$ has been replaced by unity, instead of the actual hamiltonian H; i.e. that $\frac{\partial}{\partial r} r$ is not interchangeable with the summation. The correct calculation with the correct pseudopotential gives, instead of the expression

$$\Sigma'\left[k^2 + k_o^2 - \sqrt{k^4 + 2k_o^2 k^2}\right] ,$$

the following:

$$\left[\frac{\partial}{\partial r} r \, \Sigma' e^{i\vec{k}\cdot\vec{r}}\left[k^2 + k_o^2 - \sqrt{k^4+2k_o^2k^2}\right]\right]_{r=0} = \sum_k{}'\left[k^2 + k_o^2 - \sqrt{k^4+2k_o^2k^2} - \frac{k_o^4}{2k^2}\right]$$

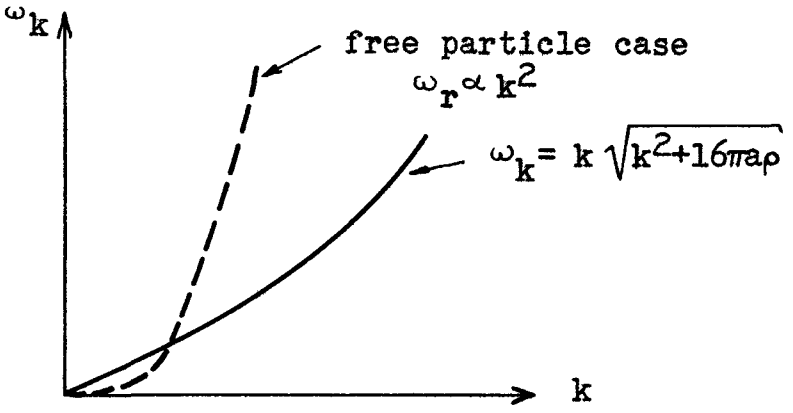
which converges to give a contribution $4\pi a\rho \, N \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3}$ to the ground state energy.

Therefore

$$\frac{H''}{N} = 4\pi a\rho \left[1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3}\right] + \sum_k \sqrt{k^4 + 2k_o^2 k^2} \; b_k^* b_k \qquad (7.17)$$

The excitation energy is

$$\omega_k = \sqrt{k^4 + 16\pi a\rho k^2} = k\sqrt{k^2 + 16\pi a\rho}$$



We see that for small k

$$\omega_k \cong k \sqrt{16\pi a\rho}$$

i.e. linear function of k charactheristic of phonon excitations: sound waves with velocity

$v = \sqrt{16\pi a\rho}$ in a medium of density ρ.

Compression waves in the ground state

The velocity of the compression waves can be obtained from the following. For a medium in the ground state, the pressure is given by

$$P = \frac{-\partial E}{\partial \Omega} = -\frac{\partial}{\partial \Omega}\left[4\pi a \frac{N}{\Omega} N\right] = 4\pi a \frac{N^2}{\Omega^2} = 4\pi a \rho^2$$

Upon compression, waves are produced, the velocity of which is given by

$$v = \sqrt{\frac{\partial P}{\partial \rho_m}}$$

ρ_m : mass density. In this case, as $2m = 1$, $\rho_m = \frac{1}{2}\rho$. Therefore

$$v = \sqrt{\frac{\partial P}{\partial(\frac{1}{2}\rho)}} = \sqrt{16\pi a\rho}$$

as obtained before from $\omega_k = \sqrt{k^4 + 16\pi a\rho k^2}$ in the limit of small k.

Dependence on N of the energy

Again, the ground state energy is given by:

$$E_{gd} = 4\pi a\rho(N-1) - \sum_k{}' \left[k^2 + k_o^2 - \sqrt{k^4 + 2k_o^2 k^2} - \frac{k_o^4}{2k^2}\right] \qquad (7.18)$$

where $k_o = \sqrt{8\pi a\rho}$. We can expand in power series in terms of a and compare with the perturbation expansion, section 6, for the Bose system:

$$\frac{E_{gd}}{N} - 4\pi a\rho = \frac{1}{N} \sum_k{}' \left[k^2 + k_o^2 - \sqrt{k^4 + 2k_o^2 k^2} - \frac{k_o^4}{2k^2}\right] = \frac{\text{const.}}{N} \sum_k{}' \frac{k_o^6}{k^4} + \ldots$$

$$= \text{const.} \frac{a^3\rho^3}{N} \sum_k{}' \frac{1}{(\ell^2+m^2+n^2)^2} \frac{1}{\left(\frac{2\pi}{L}\right)^4} + \ldots \quad (7.19)$$

This term is clearly recognizable in the expansion of Section 6. If we consider the additional terms in (7.19) we obtain

$$\frac{E_{gd}}{N} - 4\pi a\rho = \text{const.} \frac{1}{NL^2} \left[\left(\frac{aN}{L}\right)^3 + \text{const.} \left(\frac{aN}{L}\right)^4 + \ldots\right]$$

Sucessive terms differ by order of $\frac{aN}{L}$ as in the perturbation expansion. Let $x = \frac{aN}{L}$ and write

$$\frac{E_{gd}}{N} - 4\pi a\rho = \text{const.} \frac{1}{NL^2} f(x)$$

If we assume $f(x) \sim x^\alpha$ in the limit $x \to \infty$, let us determine what value of α will make the above expression finite, i.e.

$$\frac{1}{NL^2}\left(\frac{aN}{L}\right)^\alpha = \text{finite}$$

then

$$\frac{1}{NL^2}\left(\frac{aN}{L}\right)^\alpha = a^\alpha \rho^{\alpha+1} \frac{L^{2\alpha+1}}{N^2} \Longrightarrow \begin{array}{l} 2\alpha+1 = 6 \\ \therefore \alpha = \frac{5}{2} \end{array}$$

and

$$\frac{1}{NL^2}\left(\frac{aN}{L}\right)^{5/2} = a^{5/2} \rho^{3/2} = a\rho\sqrt{\rho a^3}$$

This is precisely the first order correction in eq. (7.17).

If we consider the contribution of the terms of the type $(0,k_1)\to(k_2,k_3)$ which were neglected in the computation of (7.17) we can show that this contribution is of the form

$$\frac{1}{NL^2}\left[\frac{a^3N^3}{L^3} + \text{const.}\ \frac{a^4N^3}{L^4} + \dots\right] = \frac{1}{N^2L^2}\ g\ (x)$$

The requirement for convergence as $x\to\infty$ is $g(x)\sim x^\beta$ with $\beta = 4$. The result is proportional now to $a\rho\ (\sqrt{\rho a^3})^2$ and differs from the first order correction by the factor $\sqrt{\rho a^3}$.

These arguments illustrate that the perturbation expansion can be rearranged to yield a finite result if the expansion parameter is taken to be $\sqrt{\rho a^3}$ instead of a, and that precisely we have found an expression for the energy (eq. (7.17)) in which the successive terms differ by order of $\sqrt{\rho a^3}$.

§8. Higher Order Calculations

(Physical Rev. 112, 1419; 115, 1390; 116, 489, 1344; Soviet Phys. JETP 7, 299).

The ground state energy has been calculated to higher orders. The result is

$$\frac{E_{gr}}{N} = 4\pi a\rho\left[1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + \delta\left(\frac{4\pi}{3} - \sqrt{3}\right)\rho a^3\ \ln\ (\rho a^3)\right.$$

$$\left. + K\rho a^3 + \text{higher order terms}\right].$$

The excitation energy of a phonon has also been calculated to higher orders.

The phonons were found to be unstable because of possible disintegrations into phonons of longer wave lengths. This was discussed in Phys. Rev. 112, 1419 and in Soviet Phys. JETP 7, 299.

§9. Dense Hard Spheres

Up to now we have considered the behaviour of a gas of very low density. Now we like to study the behaviour for high density. We are interested only in the expression for the energy for low $\frac{\Omega}{N}$. It is to be noted that here the physical situation is completely different from that for low densities because here we are in the region of very close packing, the particles are very crowded and the collisions among them are very frequent.

For N particles enclosed in a box we are faced with a 3N-dimensional problem. For each configuration of this N particles there correspondes a point in this space. To each permutation of the particles there correspond also a point and thus, for a fixed relative position of the particles there are N! different points in the configuration space. An interesting problem to consider is to determine what is the region in the configuration space whose points give an allowed configuration of the system in question.

Consider first the case in which the box has such dimensions that the particles are in the situation of closest packing, e.g.,

the particles are arranged in a closest packed face centred cubic lattice. The possible configurations of this arrangement are given by $N!$ points in the 3N-dimensional configuration space. Increasing the size of the box the particles acquire some freedom and the allowed region for the points of the system in the 3N-dimensional configuration space become small pockets around the $N!$ points that represent the closest packing situation as shown in fig. 9.1. Enlarging still the box, all these pockets become connected by very narrow channels. For almost closest packing the channels are extremely narrow and their effect may be neglected. One can give a semiquantitative argument

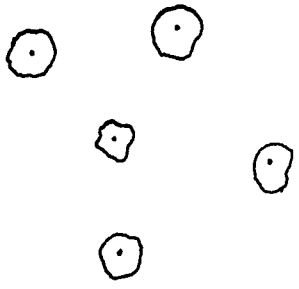


Fig. 9.1

to see under what conditions it is possible to neglect the effect of the channels; since the mean distance between the particles is of the order of $\ell = \rho^{-\frac{1}{3}}$, where ρ is the density of the system, in order to interchange two particles it is necessary to move $\sim \frac{a}{\ell - \ell_0}$ particles, a being the diameter of the hard spheres and ℓ_0 the value of ℓ for closest packing. If this number is much larger than one, i.e., if $\ell \sim \ell_0$ it is justified to neglect the influence of the channels because they are very narrow and long.

The Polyhedron Method

For the present discussion, we consider that the particles are

arranged in a simple cubic lattice.

The equations defining the allowed region in the configuration space are of the form $|\vec{r}_1 - \vec{r}_2| \geqslant a$, where $\vec{r}_1$ and $\vec{r}_2$ represent the coordinates of the center of the spheres 1 and 2 respectively. Writing in full detail this condition we get

$$\left[(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)\right]^{\frac{1}{2}} \geqslant a \qquad (9.1)$$

We can change somewhat this condition by considering small departures from the simple cubic array, (see fig. 9.2). Since in this case $y_1 - y_2$ and $z_1 - z_2$ are very small compared with $x_1 - x_2$, we may replace the above condition by $|x_1 - x_2| \geqslant a$, which is equivalent to replacing the spherical surface by its tangent plane at the point of contact of the two particles. If we do not permit interchange between the particles, the condition imposed for the x coordinates of the particles that are in the bottom row are

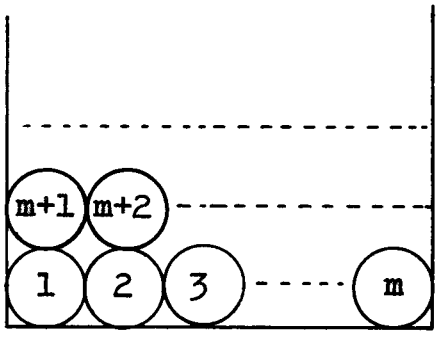


Fig. 9.2

$$x_1 \geqslant \frac{a}{2}, \; x_2 - x_1 \geqslant a, \; x_3 - x_2 \geqslant a, \; \ldots, \; x_m - x_{m-1} \geqslant a, \; x_m \leqslant L - \frac{a}{2} \qquad (9.2)$$

For the other rows we have similar systems of equations. We must add also the system of equations corresponding to the y and z components. We obtain then a system of $3\ m^2$ equations which define a polyhedron in the 3N-dimensional space.

This polyhedron is further simplied by the follwoing displacement transformation:

$$x_j' = x_j + \frac{a}{2} - ja \qquad (9.3)$$

Then

$$0 \leqslant x_1' \leqslant x_2' \quad \ldots \quad \leqslant x_m' \leqslant L - m\,a \qquad (9.4)$$

The wave function is a product of $3\ m^2$ wave functions for the various rows and columns. The wave function for the first row, $\psi\ (x_1', \ldots x_m')$, satisfies the condition that $\psi = 0$ on the boundary of the region defined by eqs. (9.4).

Now consider an antisymmetrical wave function φ of m free particles x_j' $(j = 1,2, \ldots m)$ in one dimension in a section of length L - ma. Clearly φ satisfies the same equations, and satisfy the same boundary conditions on the polyhedron defined by eqs. (9.4) One thus obtains the following theorem:

<u>Theorem</u>: The energy levels of the m^3 spheres near a simple cubic arrangement are approximately those of a collection of $3\ m^2$ independent system each of which is a Fermi system of free one-dimensional particles confined in a length L-ma.

For the calculation of the ground state energy, we first take one of the $3m^2$ systems. For this system of Fermions, the momentum goes from $-P$ to $+P$. This momentum is related to the length of the box and to the number of particles in the row by

$$\frac{2P(L - ma)}{2\pi} = m$$

and so

$$P = \frac{\pi m}{L - ma} = \frac{\pi}{\frac{L}{m} - a} \tag{9.5}$$

The energy for a row is thus given by

$$m \frac{\int_{-P}^{+P} P^2 \, dP}{\int_{-P}^{+P} dP} = m \frac{\frac{2}{3} P^3}{2P} = \frac{m}{3} P^2 \tag{9.6}$$

The total energy is equal to the energy of a row multiplied by $3m^2$. Total energy for the ground state of the system.

$$E_{gr} = 3m^2 \frac{mP^2}{3} = NP^2 = N \frac{\pi^2}{\left(\frac{L}{m} - a\right)^2} \tag{9.7}$$

Since the total number of particles is equal to m^3.

We like now to compare this result with that obtained by the cell theory. In the cell theory each particle is confined to be in a cube of side length L/m and is not allowed to be out of this

cube. The center of the sphere is then confined to a smaller cube of side length $\frac{L}{m} - a$. For the x coordinate the wave function for the particle inside the cube is given by

$$\sin \frac{\pi}{\frac{L}{m} - a} x$$

The energy for one particle, taking into account the three degrees of freedom is then

$$3 \frac{\pi^2}{(\frac{L}{m} - a)^2}$$

The total energy for the system of N particles is

$$E_{gr} = N \frac{3\pi^2}{(\frac{L}{m} - a)^2} \qquad (9.8)$$

It is to be noted that this energy is larger by a factor 3 than that obtained by the polyhedral method, eq. (9.7). The reason for this difference is that in the latter method we have more freedom to move the particles, since the only constraint imposed is that one is not allowed to interchange the particles in a row.

<u>Excited States</u>: The theorem quoted above shows that the excited states near the ground state have the structure of that of a system of Fermions. This is <u>qualitatively different</u> from the case for a dilute system discussed previously.

<u>Face centred cubic arrangement</u>.

This situation is that of a closest packing. The simple cubic

arrangement will decay through the channels into the face centred cubic lattice (see fig. 9.3).

One can use in this case also the polyhedron method although it is not easy to write down the equations as in the previous case.

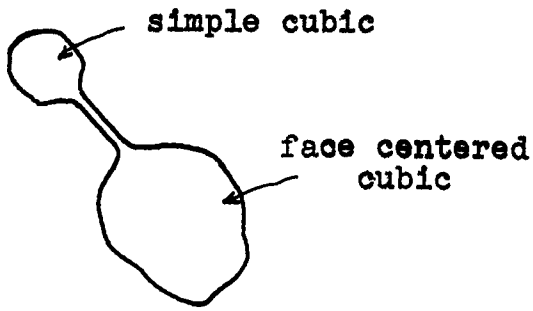


Fig. 9.3

For the x coordinate of the particles in the bottom row there exists the same kind of relations that were settled for the simple cubic lattice. One of the restrictions imposed upon the coordinates of particles 1 and m (see fig. 9.4) is given by

$$\frac{1}{2}(x_m - x_1) + \frac{\sqrt{3}}{2}(y_m - y_1) \geqslant a$$

The application of the polyhedral method to the simple cubic lattice was succesful because the method of images could be applied to obtain the wave function of the system. This is very useful if the hyper-planes defining the polyhedrons form angles that are integer divisors of 2π.

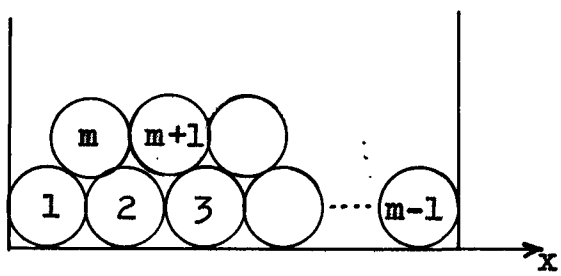


Fig. 9.4

For example, in the case of the simple cubic lattice, let us find the angles between two planes of the polyhedron where the x_j' are defined in terms of x_j by eq. (9.3).

Equation of the plane in normal coordinates	Components of the normal to the plane						
	.....		x_3'	x_2'	x_1'	.....	
$\frac{1}{\sqrt{2}}(x_3' - x_2') = 0$	0	0	$1/\sqrt{2}$	$-1/\sqrt{2}$	0	0	...
$\frac{1}{\sqrt{2}}(x_2' - x_1') = 0$	0	0	0	$1/\sqrt{2}$	$-1/\sqrt{2}$	0	...

The angle θ formed by the two planes is such that $\cos\theta = -1/2$, i.e., $\theta = 60^\circ$ which is the sixth part of 2π. Then one can apply the image method in a straightforward way, as we did.

In the present case we have

Equation of the plane	Components of the normal						
	...	x_2'	x_1'	x_m'	y_m'	y_1'	...
$\frac{1}{\sqrt{2}}(x_2' - x_1') = 0$	...	$1/\sqrt{2}$	$-1/\sqrt{2}$	0	0	0	...
$\frac{1}{\sqrt{8}}(x_m' - x_1') + \frac{\sqrt{3}}{8}(y_m' - y_1') = 0$	...	0	$-1/\sqrt{8}$	$1/\sqrt{8}$	$\sqrt{3}/8$	$\sqrt{3}/8$	0 ...

The angle formed by these two surfaces is such that $\cos\theta = 1/4$. This angle is not submultiple of 2π. Here one can perhaps use the method of multiple images but the problem turns out to be extremely difficult to solve. Although there is not yet an answer to this problem, one may expect that the expression for the energy of the system has the form

$$E = N \frac{\alpha}{(\rho^{-1/3} - \rho_0^{-1/3})} \qquad (9.9)$$

where ρ is the actual density of the system, ρ_0 is the density of the closest packing and α is an unknown constant.

Soft spheres

The potential in this case is of the form given in fig. 9.5 a) and b).

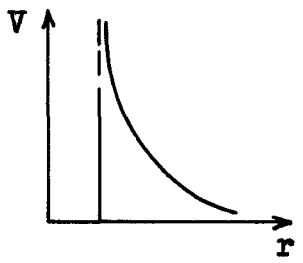


Fig. 9.5 a)

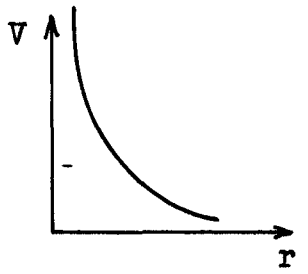


Fig. 9.5 b)

The problem may be tackled using a variational method. It can be shown that if the potential raises faster than $1/r^2$, the energy per particle is asymptotically of the form

$$6V(\ell)$$

where ℓ is the distance between the atoms in a face centred cubic lattice.

§10. Incomplete Macroscopic Occupation of Single-particle Ground State.

In the computations we made, we started from the single-particle wave functions, and by repeated applications of the off--diagonal elements we got the true ground-state. Also, we replaced

for instance the term $a_o^* a_o^* a_i a_j$ by $\sqrt{n_o^2}\ a_i a_j$ (or $n_o a_i a_j$, simply).

For our present purpose, we want to apply the approximation method used before to the states for which there is macroscopic but <u>incomplete</u> occupation of the single-particle ground state. Thus, we set the single-particle ground state occupation number

$$n_o = N\xi \tag{10.1}$$

where ξ denotes a finite fraction. It is also assumed that there are <u>numerous</u> other states occupied, yet none of them <u>alone</u> is occupied by a <u>finite</u> fraction of N. That is to say, we assume here n_i $(i \neq 0)$ are all small but there are numerous i's, so that only the sum $\sum_{i\neq 0} n_i$ gives a finite fraction of N.

Let us take a <u>particular</u> state of this kind:

$$\Sigma' \overset{o}{n}_i + \overset{o}{n}_o = N \tag{10.2}$$

where the prime over the summation sign means that i = 0 is excluded and where the superscripts "0" denotes our <u>particular</u> state. Next, we write down a small deviation of the occupations as

$$\Sigma' \overset{1}{n}_i + \overset{1}{n}_o = 0 \tag{10.3}$$

where the superscripts "1" denotes the deviation from the state "0". It is assumed here that both $\overset{1}{n}_i$ and $\overset{1}{n}_o$ are small. The actual state of interest is thus given by:

$$\begin{aligned} n_o &= \overset{o}{n}_o + \overset{1}{n}_o \\ n_i &= \overset{o}{n}_i + \overset{1}{n}_i \end{aligned} \tag{10.4}$$

1) <u>The diagonal elements</u>; they are (see eq. (5.9)):

$$\frac{4\pi a}{\Omega}\left[2N^2 - N - \Sigma n_i^2\right]$$

$$= \frac{4\pi a}{\Omega}\left[2N^2 - N - \sum_i{}' n_i^2 - n_o^2\right]$$

$$= \frac{4\pi a}{\Omega}\left[2N^2 - N - \sum_i{}' (\overset{o}{n}_i + \overset{1}{n}_i) - (\overset{o}{n}_o + \overset{1}{n}_o)^2\right]$$

$$= \frac{4\pi a}{\Omega}\left[2N^2 - N - \sum_i{}' \overset{o}{n}_i{}^2 - 2\sum_i{}' \overset{o}{n}_i \overset{1}{n}_i - \sum_i{}' \overset{1}{n}_i{}^2 - n_o^2 + 2\overset{o}{n}_o \sum_i{}' \overset{1}{n}_i - \left(\sum_i{}' \overset{1}{n}_i\right)^2\right]$$

the terms $-N - \sum_i{}' \overset{o}{n}_i{}^2$ are numerical constants much smaller than N^2. They will be neglected. The terms $-2\Sigma' \overset{o}{n}_i \overset{1}{n}_i - \Sigma' \overset{1}{n}_i{}^2 - (\Sigma' \overset{1}{n}_i)^2$ are also negligible.

Thus we have

$$|\text{diagonal elements}| \cong \frac{4\pi a}{\Omega}\left[2N^2 - \overset{o}{n}_o{}^2 + 2\overset{o}{n}_o \sum_i{}' \overset{1}{n}_i\right]$$

$$= \frac{4\pi a}{\Omega}\left[2N^2 - (N\xi)^2 + 2(N\xi)\sum_i{}' (n_i - \overset{o}{n}_i)\right]$$

$$= \frac{4\pi a}{\Omega} N^2 \left[2 - \xi^2 - 2\xi(1-\xi)\right] + \frac{4\pi a}{\Omega} 2N\xi \sum_i{}' n_i$$

$$= 4\pi a\rho N\left[1 + (1-\xi)^2\right] + 8\pi a\rho\xi \sum_i{}' n_i$$

obviously, if we put $\xi = 1$ we shall get exactly the same result as we got for the case of complete occupation of the ground state (see eq. (7.9)).

ii) <u>The off-diagonal elements</u>; as before they are divided into classes according to the power of a_o and a_o^*. The largest off--diagonal elements are those of

$$a_o^* a_o^* \, a_k a_{-k}$$

and

$$a_k^* a_{-k}^* a_o a_o$$

The off-diagonal elements, thus, will take the form

$$\frac{4\pi a}{\Omega} \left[\sum_k a_k^* a_{-k}^* N\xi + \sum_k N\xi \, a_k a_{-k} \right]$$

where we have replaced $a_o^* a_o^*$ and $a_o a_o$ by $N\xi$.

iii) <u>The total Hamiltonian</u>, will take the form

$$H'' = 4\pi a\rho N \left[1 + (1-\xi)^2\right] + \sum_k{}' (k^2 + 8\pi a\rho\xi) \, a_k^* a_k +$$

$$+ 4\pi a\rho\xi \sum_k{}' (a_k^* a_{-k}^* + a_k a_{-k}) \qquad (10.5)$$

again, it is obvious, if we set $\xi = 1$ the Hamiltonian will be reduced to the same one used before for the case of complete occupation, eq. (7.11).

By means of the same Canonical transformation we used before (eq. (7.12)) we can write the Hamiltonian in terms of operators

b_k^* and b_k:

$$H'' = 4\pi a\rho N \left[1 + (1-\xi)^2 + (128/15\sqrt{\pi})\sqrt{\rho a^3}\,\xi^{5/2}\right]$$

$$+ \sum_k{}' \left(k^4 + 16\pi a\rho\xi k^2\right)^{\frac{1}{2}} b_k^* b_k \tag{10.6}$$

where the last term gives the excitations.

The number of excitation is approximately given by

$$\sum_k{}' b_k^* b_k = N(1-\xi) \tag{10.7}$$

and we may sepparate the total energy of the system into two parts, namely

$$E(\xi, m_k) = E_o(\xi) + E_{phonon}(\xi, m_k) \tag{10.8}$$

where the ground state energy is given by

$$E_o(\xi) \equiv 4\pi a\rho N \left[1 + (1-\xi)^2 + (128/15\sqrt{\pi})\sqrt{\rho a^3}\,\xi^{5/2}\right] \tag{10.9}$$

and the total energy of the excited phonons is given by

$$E_{phonon}(\xi, m_k) \equiv \sum_k{}' m_k \left(k^4 + 16\pi a\rho\xi k^2\right)^{\frac{1}{2}} \tag{10.10}$$

and $\sqrt{16\pi a\rho\xi}$ is the phonon velocity (cf. the discussion after eq. (7.17)). Attention should be paid to the fact that the m_k's are subject always to the condition

$$(1/N)\sum_k{}' m_k = 1 - \xi \tag{10.11}$$

It is easy to verify that the total momentum of the system in the state specified by ξ, m_k is given by

$$\vec{P}(\xi, m_k) = \Sigma \vec{k}\, a_k^* a_k = \Sigma \vec{k}\, m_k \qquad (10.12)$$

where m_k is the number of excited phonons with momentum $\vec{k}$.

Related Discussions:

Concerning the previous calculation we would like to make the following remarks:

a) The relationship between degenerate occupation of a single--particle ground state and the number of phonon excitations.

Equation (10.11) says that the number of excited phonons is equal to the degeneracy of the occupation of the single-particle ground state, which is an important result since it establishes a relationship between the degeneracy of the occupation of the single--particle ground state, a concept already discussed by London, and the number of phonon excitations, a concept discussed by Landau.

b) Order of Accuracy of the Calculation

For the ground state,

$$E_o(\xi) = 4\pi a\rho N\left[1 + (1-\xi)^2 + (128/15\sqrt{\pi})\sqrt{\rho a^3}\,\xi^{5/2}\right] + 0(\rho a^3 N) \qquad (10.13)$$

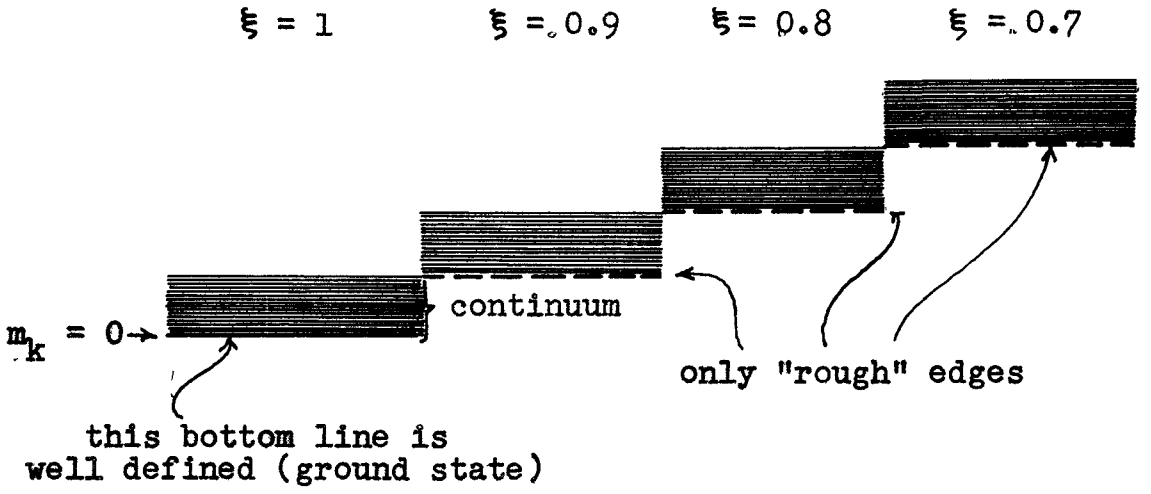
For the phonon state,

$$E_{phonon}(\xi, m_k) = \sum_k{}' m_k(k^4 + 16\pi a\rho\xi k^2)^{\frac{1}{2}} + 0(\sqrt{\rho a^3}N) \qquad (10.14)$$

Notice, however that the energy $\omega_k = (k^4 + 16\pi a\rho\xi k^2)^{\frac{1}{2}}$ of each phonon is accurate to the order of N^0 and not N^1.

c) <u>Computational Separation of the Hamiltonian into Different Regions</u>.

One interesting aspect is the separation of the Hamiltonian into different regions for computational purpose. Such a separation is certainly not well-defined, therefore we might ask ourselves what is the criterion. The situation is like that shown below:



The different Hamiltonians specified by different ξ's represent approximations to the true Hamiltonian in different regions of energy. This is quite similar to the discussion of §9 where we saw that the approximate energy levels in different pockets (face centred cubic, simple cubic etc.) collectively give the energy levels of the system.

§11. Thermodynamic Properties of a Dilute Hard-sphere Bose system.

Ref. Phys. Rev. 112, 1419

According to statistical mechanics, all the thermodynamic functions can be obtained once we get the partition function of the system. This partition function Q is defined by

$$Q = \sum_{m,\xi} e^{-\beta E(m,\xi)} \tag{11.1}$$

where $\beta = 1/KT$ and K is the Boltzmann constant and T the absolute temperature. Here "m" denotes the set $m_1, m_2, \ldots$ for different combinations of occupations. The values of the m_k's are subject always to the condition

$$(1/N) \sum_k{}' m_k = 1 - \xi \, . \tag{11.2}$$

Now introduce the partial partition function, $Q(\xi)$ defined by

$$Q(\xi) \equiv \sum_m e^{-\beta E(m,\xi)} \tag{11.3}$$

where the sum over m is subjected to condition (11.2). We have now, in partial partition sum

$$Q = \sum_\xi Q(\xi) \tag{11.4}$$

Substitution of the energy eigenvalue into the partial partition function leads to

$$\begin{aligned} Q(\xi) &= \sum_m e^{-\beta E_o(\xi)} \; e^{-\beta \sum_k m_k \omega_k} \\ &= e^{-\beta E_o(\xi)} \sum_m e^{-\beta \sum_k m_k \omega_k} \end{aligned} \tag{11.5}$$

where $E_o(\xi)$ is given by eq. (10.9), the m_k's are subject to condition (11.2) and ω_k is defined by

$$\omega_k \equiv (k^4 + 16\pi a \rho \xi k^2)^{\frac{1}{2}} \tag{11.6}$$

Next, let us introduce the function

$$R\ (M) \equiv \sum_m e^{-\beta \sum_k m_k \omega_k} \tag{11.7}$$

where m_k is subject to the condition

$$\sum_k m_k = M \tag{11.8}$$

We may introduce another function Q, the generating function for Q, defined by

$$Q \equiv \sum_{M=0}^{\infty} \zeta^M R\ (M) \tag{11.9}$$

where ζ is a complex number. Now we can write

$$Q = \sum_m e^{-\beta \sum_k m_k \omega_k} \zeta^{\sum_k m_k} \tag{11.10}$$

without condition on the m's, or

$$Q = \prod_k (1 - \zeta e^{-\beta \omega_k})^{-1} \tag{11.11}$$

Now we shall be interested only in $\ln Q$ and especially in the limit $N \to \infty$. In this case only one term in the sum (11.9) <u>predominates</u> the logarithm of the sum. Thus, we have the asymptotic approximation of (11.9):

$$\ln Q = \bar{M} \ln \zeta + \ln R(\bar{M}) \tag{11.12}$$

where $\bar{M}$ denotes the value of M of the dominating term.

Differentiation of (11.12) with respect to M yields immediately

$$\ln \zeta + \frac{d}{dM} \ln R(\bar{M}) = 0 \tag{11.13}$$

On the other hand, with (11.11) into the left side of (11.12), we get

$$- \sum_k \ln (1 - \zeta e^{-\beta\omega_k}) = \bar{M} \ln \zeta + \ln R(\bar{M}) \tag{11.14}$$

Differentiating the last equation with respect to $\ln \zeta$ we obtain

$$\sum_k \frac{\zeta e^{-\beta\omega_k}}{1 - \zeta e^{-\beta\omega_k}} = \bar{M} + \left[\ln \zeta + \frac{d}{d\bar{M}} \ln R(\bar{M})\right] \frac{dM}{d\ln\zeta}$$

which is simplified, by means of (11.13), to

$$\bar{M} = \sum_k \frac{\zeta e^{-\beta\omega_k}}{1 - \zeta e^{-\beta\omega_k}} \tag{11.15}$$

Now we may list all the formulae

i) Free energy $\quad F = - kT \ln Q \quad$ (11.16)

ii) Logarithm of the partition function: $\quad \ln Q = [\ln Q(\xi)|_{\max.w.r.t.\xi}$ (11.17)

iii) The partial partition function: $\quad Q(\xi) = e^{-\beta E_o(\xi)} R[N(1-\xi)]$ (11.18)

iv) $$\ln R(M) = - \sum_k \ln (1 - \zeta e^{-\beta\omega_k}) - M \ln \zeta \tag{11.19}$$

(here we dropped the bar over M for simplycity of notation)

v) $$M = \sum_k \frac{\zeta e^{-\beta\omega_k}}{1 - \zeta e^{-\beta\omega_k}} \tag{11.20}$$

where

$$\omega_k = k\,(k^2 + 16\pi a\rho\xi)^{\frac{1}{2}} \tag{11.21}$$

and M (i.e. $\bar{M}$) is obviously the most probable total number of excitations in the system.

The above equations (11.16) - (11.21) allow for a computation of F. We are not going into the exposition of the detailed calculations; instead let us discuss some of the results of the calculation:

i) <u>The T - p plot</u>

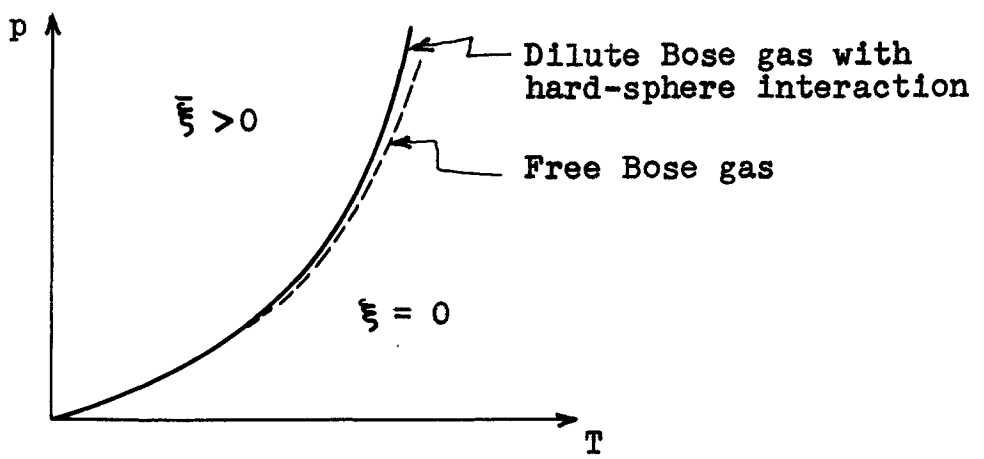
We find the transition curve as

$$\lambda^3 p_c/kT = 1.342 + 2(2.612)^2\,(a/\lambda) + 0\left[(a/\lambda)^{3/2}\right]$$

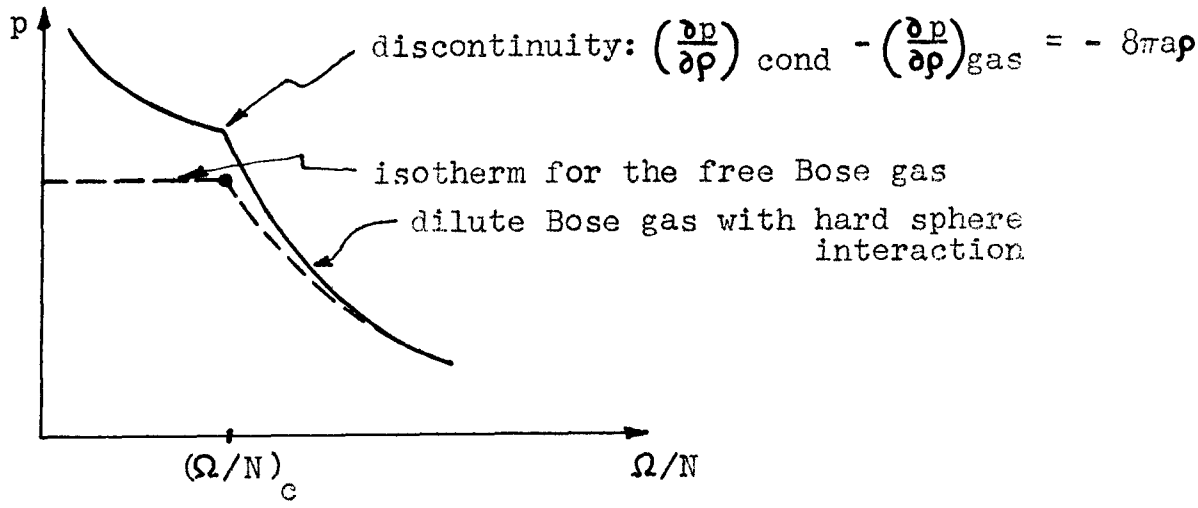
and

$$\lambda^3 p_c = 2.612 + 0\,(a/\lambda)$$

where the subscript c denotes the transition point, and λ the thermal De Broglie wavelength $(4\pi/kT)^{\frac{1}{2}}$.



ii) The p - V diagram



§12. Two-Fluid Motion Ref.: Phys. Rev. 113, 1406

a) Galilean Transformation

Taking the system of a dilute Bose hard spheres and using a Galilean transformation to such a system we can get a new eigenstate in which there is a macroscopic occupation of a single-particle state with $\vec{k} \neq 0$.

Let the transformation be defined by a relative velocity $\vec{v}$, and the primed stand for the system in which condensation occurs at $\vec{k} = 0$ while the unprimed notation stand for the system in which condensation occurs at $\vec{k} = \vec{k}_s$ ($\neq 0$).

Thus, in the laboratory system (unprimed system) of coordinates $\vec{k}_s \neq 0$, the total momentum of the system is

$$\vec{P} = (\text{mass}) \cdot \vec{v} + \vec{P}' \tag{12.1}$$

and the energy is

$$E = \tfrac{1}{2}\,(\text{mass})\,v^2 + \tfrac{1}{2}\;2\,\vec{v}.\vec{P}' +$$

$$+ \text{ energy in the moving system.} \qquad (12.2)$$

By previous convention: (particle mass) = $\frac{1}{2}$; thus

$$\vec{P} = \tfrac{1}{2}\,N\vec{v} + \sum_q{}' \, m_q \, \vec{q} \qquad (12.3)$$

where $\vec{q}$ is the momentum of the phonons with respect to the moving system, and the primed summation denotes the exclusion of $\vec{q} = 0$ as before.

Now, the energy from (12.2) can be written as

$$E = \tfrac{1}{2}\left(\frac{N}{2}\right) v^2 + \vec{v}.\sum_q{}' \, m_q \, \vec{q} +$$

$$+ 4\pi a\rho N\left[1 + (1-\xi)^2\right] + \sum_q{}' m_q \left(q^4 + 16\pi a\rho\xi q^2\right)^{\frac{1}{2}}. \qquad (12.4)$$

By setting (remember that the particle mass is taken to be $\frac{1}{2}$):

$$\vec{k}_s \equiv \tfrac{1}{2}\,\vec{v} \qquad (12.5)$$

we can rewrite the expressions as

$$\vec{P} = N\vec{k}_s + \sum_q{}' \, m_q \, \vec{q} \qquad (12.6)$$

$$E = N\,k_s^2 + \sum_q{}' \, m_q \left(2\vec{k}_s.\vec{q} + \omega_q\right) + 4\pi a\rho N\left[1 + (1-\xi)^2\right] \qquad (12.7)$$

$$(1/N) \sum_q{}' \, m_q = 1 - \xi \qquad (12.8)$$

$$\omega_q = \left(q^4 + 16\pi a\,\rho\,\xi\,q^2\right)^{\frac{1}{2}} \qquad (12.9)$$

We can also write (12.6) as

$$\vec{P} = N\xi\vec{k}_s + N(1-\xi)\vec{k}_s + \sum_q{}' m_q \vec{q}$$

$$= N\xi\vec{k}_s + \sum_q{}' m_q (\vec{q} + \vec{k}_s) \qquad (12.10)$$

b) <u>The Quantum Numbers ξ, m_q, $\vec{k}_s$</u>

These parameters ξ, m_q, k_s are not absolute quantum numbers due to the fact that, for instance, phonons may decay or scatter among themselves. They are good quantum numbers only if these effects are small enough to be treated as small perturbations. Among these three quantum numbers, however, $\vec{k}_s$ is most stable and in this sense we might consider it as a quasi-quantum number (though it is evidently physically not absolute). m_q is the most unstable one since it is affected easily by decays or collisions. ξ is rather stable, being subject to alterations only if a finite fraction of phonons suffer decays or recombinations.

c) <u>Quasi equilibrium Distribution</u>

This calculations is based on the assumption that condensation occurs at $\vec{k} \neq 0$. The previous results are summarized in (12.7) to (12.10). Now we are interested to know that if N, Ω, $\vec{k}_s$, $\vec{P}$, T are fist given then what will be the values of $\bar{m}$, $\bar{\xi}$ and F after a long time.

First, we have

$$\ln Q = \left[\ln Q(\xi, \vec{k}_s, \vec{P}) \right]_{\max. \text{ w.r.t. } \xi} \tag{12.11}$$

where

$$Q(\xi, \vec{k}_s, \vec{P}) \equiv \sum_{\underline{m}} e^{-\beta E(\xi, m, \vec{k}_s)} \tag{12.12}$$

subject to the conditions:

$$\begin{cases} \sum_q{}' \; m_q = N(1-\xi) \\ \sum m_q \vec{q} = \vec{P} - N\vec{k}_s \end{cases} \tag{12.13}$$

Next, we define

$$R(M, \vec{S}) \equiv \sum_{\underline{m}} e^{-\beta \Sigma m_q \omega_q} \tag{12.14}$$

where M and $\vec{S}$ are defined by

$$\sum_q m_q = M \tag{12.15}$$

and

$$\sum_q m_q \vec{q} = \vec{S} \tag{12.16}$$

Introduce the function $\mathcal{R}$ defined by

$$\mathcal{R} \equiv \sum_{\underline{m}} e^{-\beta \Sigma' m_q \omega_q} \zeta^{\Sigma' m_q} \xi_x^{\Sigma' m_q q_x} \xi_y^{\Sigma' m_q q_y} \xi_z^{\Sigma' m_q q_z} \tag{12.17}$$

or

$$\mathcal{R} = \prod_q{}' \left(1 - \zeta \, e^{-\beta(\omega_q - \vec{u}\cdot\vec{q})}\right) \tag{12.18}$$

where u_j is defined by

$$e^{\beta u_j} \equiv \xi_j \tag{12.19}$$

Taking the logarithm of (12.17) and neglecting small contributions except for the term <u>maximized with respect to M and $\vec{S}$</u> (this will be denoted by $\mathcal{M}$) one obtains

$$\ln \mathcal{R} = \left[\ln R\,(M,\vec{S}) + M \ln \zeta + \beta \vec{S}\cdot\vec{u}\right]_{\mathcal{M}} \tag{12.20}$$

which, under maximization, results in the following conditions

$$\ln \zeta + \frac{\partial}{\partial M} \ln R(M,\vec{S}) = 0 \tag{12.21}$$

and

$$\beta\vec{u} + \frac{\partial}{\partial \vec{S}} \ln R(M,\vec{S}) = 0 \tag{12.22}$$

By taking the logarithm of (12.18) and equating it to (12.20) we get

$$-\sum_q \ln\left[1 - \zeta\, e^{-\beta(\omega_q - \vec{u}\cdot\vec{q})}\right] = \left[\ln R(M,\vec{S}) + M\ln\zeta - \beta\vec{S}\cdot\vec{u}\right]_{\mathcal{M}} \tag{12.23}$$

Partial differentiation of (12.23) with respect to $\ln \zeta$ leads to

$$\sum_q \frac{\zeta\, e^{-\beta(\omega_q - \vec{u}\cdot\vec{q})}}{1 - \zeta\, e^{-\beta(\omega_q - \vec{u}\cdot\vec{q})}} = M = N\,(1-\xi) \tag{12.24}$$

which gives the most probable number of total phonons <u>off</u> the condensation.

On the other hand, a partial differentiation of (12.23) with respect to $\vec{u}$ leads to

$$\sum_q \frac{\zeta\, e^{-\beta(\omega_q - \vec{u}\cdot\vec{q})}}{1 - \zeta\, e^{-\beta(\omega_q - \vec{u}\cdot\vec{q})}}\,\vec{q} = \vec{S} = \vec{P} - N\,\vec{k}_s \tag{12.25}$$

which gives the most probable total momentum of the phonon clouds. Obviously, now we are able to compute ζ and $\vec{u}$ by means of (12.24) and (12.25) once ξ, $\vec{P}$, $\vec{k}_s$ are given.

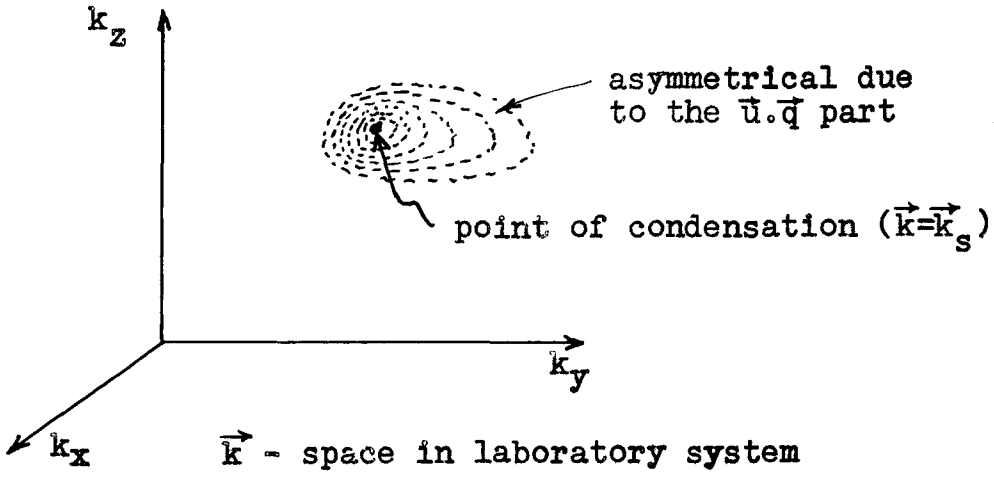
d) <u>Physical Picture of the distribution</u>

From (12.24) we can define the average value of excitations as

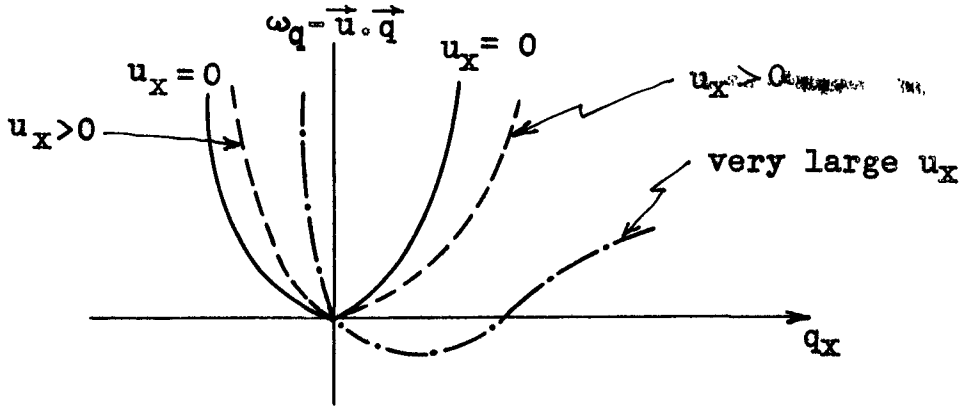
$$\bar{m}_q \equiv \frac{\zeta\, e^{-\beta(\omega_q - \vec{u}\cdot\vec{q})}}{1 - \zeta e^{-\beta(\omega_q - \vec{u}\cdot\vec{q})}} \qquad (12.26)$$

where ζ and $\vec{u}$ are determined by means of (12.24) and (12.25) while ξ is in turn determined through a maximization of (12.20).

The dependence of $\bar{m}_q$ on $\vec{k} = \vec{q} + \vec{k}_s$ gives the number of excitations with momentum $\vec{k}$ in the laboratory system. This distribution is spherically symmetrical around $k = k_s$ if $u = 0$.



Let us now look into a simple situation in which u_y and u_z are zero; thus we can plot the following curves:



The minimum of these curves gives the point at which $\bar{m}_q$ reaches a maximum, which should be at $q = 0$. The curve for very large u_x is thus unphysical. The following restriction is necessary

$$|\vec{u}| < (16\pi a \rho \xi)^{\frac{1}{2}} \qquad (12.27)$$

e) <u>Two-Fluid Motion</u>

We have seen that for a quasi-stationary state there are two degrees of freedom described by $\vec{P}$ and $\vec{k}_s$ which are analogous to a two-fluid motion. For instance, $\vec{P} = 0$, corresponds to a liquid with no total momentum but for such a system $\vec{k}_s$ may not be equal to zero. The relationship with two fluid motion is as follows:

Superfluid: $\rho_s = (1/\Omega)\, N \xi$ (12.28

Normal fluid: $\rho_n = (1/\Omega)\, N\, (1-\xi)$ (12.29)

and

$$\vec{P}/\Omega = \rho_s \vec{k}_s + \rho_n \vec{k}_n$$

$$\vec{v}_s = 2\vec{k}_s \quad .$$

$$\vec{v}_n = \vec{v}_s + \vec{u} \; .$$

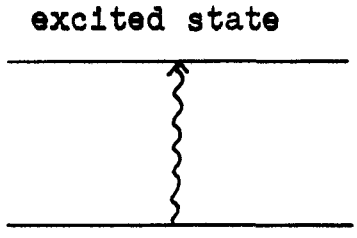
Therefore the transport phenomena may also be studied through this defined system.

f) <u>Superfluidity</u>

Now, without a detailed description, two physical concepts can be derived from the two-fluid model. For instance, let us imagine that a particle is being dragged through the system originally at $T = 0$ with no phonon excitations. The liquid after excitation has a momentum and energy given by

$$\vec{P} = \sum_k m_k \vec{k}$$

$$E = \sum_k m_k \omega_q$$



Excitation due to dragging of a particle

Now, this external particle suffers a loss of momentum and energy given by

$$\delta\vec{P} = - \sum_k m_k \vec{k}$$

$$\delta E = - \sum_k m_k \omega_k \; .$$

We have

$$|\delta E| \geqslant \sum_k m_k \, (16\pi a\rho)^{\frac{1}{2}} \, |\vec{k}| \geqslant (16\pi a\rho)^{\frac{1}{2}} \, |\delta\vec{P}|$$

or

$$\frac{|\delta E|}{|\delta \vec{P}|} \quad (16\pi a\rho)^{\frac{1}{2}}$$

thus

$$v_{ext} \geqslant (16\pi a\rho)^{\frac{1}{2}}$$

For <u>excitation</u> to become possible. Obviously, the situation is analogous to Čerenkov radiation which is possible only when the external particle has a velocity larger than a critical velocity. In our case, the fluid becomes frictionless to the particle below the critical velocity $(16\pi a\rho)^{\frac{1}{2}}$. This argument was originally due to Landau.

g) <u>Infinite Heat Conductivity</u>

The concept of infinite heat conductivity means that heat transfer is possible even in the absence of a temperature difference. Experimentally this obtains for liquid He below the λ-point. In the quasi-equilibrium state we are considering, if we set $\vec{P} = 0$ and $\vec{k}_s \neq 0$, then we have a relative motion of the super and normal fluids.

Evidently all the entropy is contained in the phonon cloud (normal fluid) thus giving rise to the possibility of a motionless ($\vec{P} = 0$) isothermal entropy flux which offers a natural explanation of such a phenomenon.

h) <u>Second Sound</u>

The addition of one more degree of freedom gives rise to the fact of two sound velocities: the first sound and the sec-

ond sound. Mathematically, it is a consequence of the existence of two different roots of the quadratic equation determining the sound velocity.

§13. General treatment of an interacting system with Bose statistics. Ref.: Phys. Rev. 113, 1165
116, 25
117, 12
117, 22
117, 897

a) Motivation

He^4 and He^3 exhibit slightly different thermodynamical behaviours. Fig. 13.1 represents schematically the phase diagram for He^4, showing the existence of two liquid phases. At the saturated vapour pressure, the transition from liquid helium I to liquid helium II occurs at approximately 2.17°K. Another feature is that at 0°K, He^4 exists as a liquid.

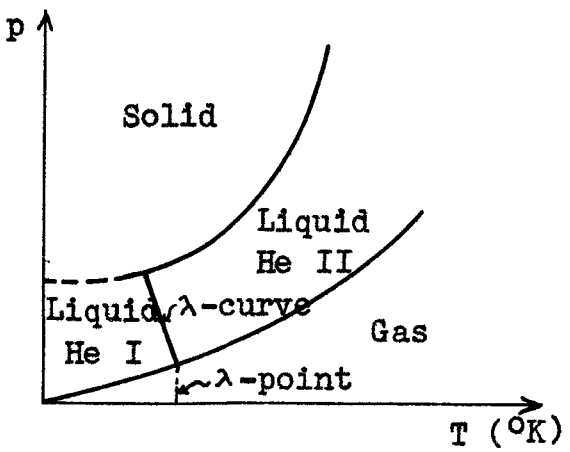


Fig. 13.1

He^3 does not exhibit a λ transition though it has been investigated down to 0.1°K. Other characteristics are similar to those of He^4. Now, since the interatomic forces are almost the same for He^3 as for He^4, the potential energy is practically the same for identical configurations. We would expect the difference in mass to intro-

duce only quantitative but not qualitative differences in the behaviours of He^3 and He^4. The absence of λ transition in He^3 and the presence of it in He^4 must then arise from the statistics.

It is our aim to show this by dealing first with the problem of the thermodynamical behaviour of a system of interacting particles with Boltzmann statistics, i.e. arbitrary statistics, and trace afterwards the effect of imposing a definite statistics. In other words, the actual problem is to be split in a part independent of statistics and a part which depends on statistics.

b) Details of the treatment

<u>Boltzmann statistics</u>

We shall follow the Ursell - Kahn - Uhlenbeck development. Introduce the density matrix:

$$\langle 1', 2', \ldots N' | W_N | 1, 2 \ldots N \rangle \equiv \langle 1', 2', \ldots N' | e^{-\beta H} | 1, 2 \ldots N \rangle \tag{13.1}$$

where

$$1 \equiv \vec{r}_1 \equiv (x_1, y_1, z_1), \text{ etc.}$$

We define a sequence of functions U_ℓ, the arguments of which involve the coordinates of ℓ particles and which have the property that they vanish rapidly when any interparticle distance in the group of ℓ particles approaches infinity, by the following relations:

$$\langle 1' | W_1 | 1 \rangle \equiv \langle 1' | U_1 | 1 \rangle$$

$$\langle 1'2' | W_2 | 1\ 2 \rangle \equiv \langle 1' | U_1 | 1 \rangle \quad \langle 2' | U_1 | 2 \rangle + \langle 1'2' | U_2 | 1\ 2 \rangle$$

$$\langle 1'2'3' | W_3 | 1\ 2\ 3 \rangle \equiv \langle 1' | U_1 | 1 \rangle \quad \langle 2' | U_1 | 2 \rangle \quad \langle 3' | U_1 | 3 \rangle$$

$$+\langle 1'|U_1|1\rangle \langle 2'3'|U_2|2\ 3\rangle \quad + \quad \langle 2'|U_1|2\rangle \langle 1'3'|U_2|\ 1\ 3\rangle$$
$$+\langle 3'|U_1|3\rangle \langle 1'2'|U_2|1\ 2\rangle \quad + \quad \langle 1'2'3'|U_3|\ 1\ 2\ 3\rangle$$

and so on. $\langle 1'|W_1|1\rangle$ is clearly the free particle distribution function. Consider now $\langle 1'2'|W_2|1\ 2\rangle$: if the two particles are very far apart, we are left with the product of free particle distribution functions, hence U_2 approaches zero. The U functions exhibit explicitly the effect of the interactions.

The general expression can be seen to be

$$W_N = \sum_{m_\ell} \sum_D \Big[\underbrace{(U_1 \ldots U_1)}_{m_1} \underbrace{(U_2 \ldots U_2)}_{m_2} \ldots \underbrace{(U_N)}_{m_N}\Big].$$
$$\sum m_\ell \ \ell = N$$

$\sum_D$ relates to all possible ways of assigning particle coordinates to the arguments of the U functions.

The partition function is by definition:

$$Q_N \equiv S_p\ W_N\ . \tag{13.4}$$

Introducing the grand partition function

$$Q = \sum_{N=0}^{\infty} (1/N!)\ Z^N\ Q_N \tag{13.5}$$

it is well known that

$$p\Omega/kT = \ell n\ Q \tag{13.6}$$

$$N/\Omega = \Omega^{-1} \frac{\partial \ell n Q}{\partial \ell n Z} \tag{13.7}$$

One can eliminate the parameter Z between these two equations and obtain the pressure as a function of the density.

In terms of the U functions:

$$Q_N = \sum_{m_\ell} \prod_{\ell=1}^{\infty} \frac{N!}{(\ell!)^{m_\ell} m_\ell!} \left[Sp(U_\ell)\right]^{m_\ell} \tag{13.8}$$

The coefficient $N!/(\ell!)^{m_\ell}\, m_\ell!$ gives the statistical weight of any particular arrangement of the N particles in m_ℓ clusters of ℓ particles each. We have then:

$$Q = \sum_{N=0}^{\infty} Z^N \sum_{m_\ell} \prod_{\ell=1}^{\infty} (Sp\ U_\ell)^{m_\ell}/(\ell!)^{m_\ell}\, m_\ell!$$

$$\Sigma \ell m_\ell = N$$

or

$$Q = \sum_{m_\ell=0}^{\infty} Z^{\Sigma \ell m_\ell} \prod_{\ell=1}^{\infty} (Sp\ U_\ell)^{m_\ell}/(\ell!)^{m_\ell}\, m_\ell!$$

$$= \sum_{m_\ell=0}^{\infty} \prod_{\ell=1}^{\infty} \left[Z^\ell\ Sp\ U_\ell/\ell!\right]^{m_\ell} (1/m_\ell!)$$

and switching sum and product:

$$Q = \prod_{\ell=1}^{\infty} \exp\left[\ Z^\ell Sp\ U_\ell/\ell!\ \right]$$

$$= \exp \sum_{\ell=1}^{\infty} Z^\ell\ Sp\ U_\ell/\ell! \tag{13.9}$$

it follows from this, (13.6) and (13.7)

$$\frac{p\Omega}{kT} = \sum_{\ell=1}^{\infty} Z^\ell\ Sp\ U_\ell/\ell! \tag{13.10}$$

$$\rho = N/\Omega = (1/\Omega) \sum_{\ell=1}^{\infty} \ell Z^\ell\ Sp\ U_\ell\ /\ell! \tag{13.11}$$

The above mathematical development is not entirely rigorous, mainly in the interchange of sum and product. However, we can assert that these equations are correct for small positive values of Z, which represent the case of low density, i.e. the gaseous state. In a more rigorous treatment, we have to confine the system in a box of volume Ω, carry out the calculations and then pass to limit $\Omega \to \infty$. Note that, as U_ℓ is a function of the relative coordinates of ℓ particles, when we perform all but one of the integrals in

$$I = \int \psi^* (1 \ldots \ell)\, U_\ell\, \psi(1 \ldots \ell)\, d\vec{1}\, d\vec{2} \ldots d\vec{\ell}$$

all variables in the integrand are exhausted, and the last integral yields only the volume Ω, i.e.

$$I = \Omega \int \psi^* (1 \ldots \ell)\, U_\ell\, \psi(1 \ldots \ell)\, d\vec{2} \ldots d\vec{\ell} \tag{13.12}$$

Substituting in eqs. (13.10) and (13.11) above, p and ρ are seen to be independent of Ω and finite in the limit $\Omega \to \infty$ if Z is small.

c) <u>Bose statistics</u>

The development is the same as in the Boltzmann case, except that the partition function is defined now as:

$$Q_N^S \equiv N! \sum_{S.S} e^{-\beta E} \tag{13.13}$$

The factor N! is introduced for convenience, and S.S. means that the sum is performed over the symmetrical states only. Then

$$\langle 1', 2', \ldots N' | W_N^S | 1, 2, \ldots N \rangle \equiv$$

$$\equiv N! \sum_{S.S} \psi_i (1', 2' \ldots N') e^{-\beta E} \psi_i^* (1, 2, \ldots N) \tag{13.14}$$

Taking the diagonal element and integrating over all coordinates, we get:

$$\mathrm{Sp}\, W_N^S = Q_N^S \tag{13.15}$$

The grand partition function is:

$$Q^S = \sum_{N=0}^{\infty} Z^N Q_N^S / N! \tag{13.16}$$

Also

$$p^S \Omega / kT = \ln Q^S \tag{13.17}$$

$$\frac{N}{\Omega} = \frac{1}{\Omega} \frac{\partial Q^S}{\partial \ln Z} \tag{13.18}$$

Again we can define some functions U^S by:

$$\langle 1' | W_1{}^S | 1 \rangle \equiv \langle 1' | U_1{}^S | 1 \rangle$$

$$\langle 1'2' | W_2{}^S | 1\, 2 \rangle \equiv \langle 1' | U_1{}^S | 1 \rangle \langle 2' | U_1{}^S | 2 \rangle + \langle 1'2' | U_2{}^S | 1\, 2 \rangle \tag{13.19}$$

etc. and proceed to obtain results analogous to the Boltzmann case.

Schematically our procedure has been the following:

$W_\ell \longrightarrow U_\ell \longrightarrow p$	Boltzmann statistics
$W_\ell{}^S \longrightarrow U_\ell{}^S \longrightarrow p^S$	Bose statistics
$W_\ell{}^A \longrightarrow U_\ell{}^A \longrightarrow p^A$	Fermi statistics

The problems that arise now are how to compute the U_ℓ functions from the interactions and how to relate to each other the different W's. We shall consider the second question.

d) <u>Relationship between Bose statistics and Boltzmann statistics</u>.

We have

$$\langle 1',2', \ldots N'|W_N{}^S|1,2 \ldots N\rangle = N!\sum_{S.S} \psi_1(1'\ldots N')\, e^{-\beta E}\, \psi_1^*(1\ldots N)$$

and

$$\langle 1',2', \ldots N'|W_N|1,2 \ldots N\rangle = \sum_{\text{all st.}} \psi_1(1'\ldots N')e^{-\beta E}\, \psi_1^*(1\ldots N)$$

In the second equation, permute the primed coordinates and sum over all permutations:

$$\sum_{P'} P'\langle 1',2'\ldots N'|W_N|\, 1,2 \ldots N\rangle =$$

$$= \sum_{\text{all st.}} \Big[\sum_{P'} P'\psi(1'\ldots N')\, e^{-\beta E}\, \psi(1 \ldots N)$$

From the sum, separate out the symmetrical states. Clearly we have:

for symmetrical states $\quad \sum_{P'} P'\psi = N!\,\psi$

for the other states $\quad \sum_{P'} P'\psi = 0$

and we get:

$$\sum_{P'} P'\langle 1', \ldots N'|W_N|\, 1 \ldots N\rangle = \langle 1'\ldots N'|W_N{}^S|\, 1\ldots N\rangle \tag{13.20}$$

The program to follow is then:

$$U_\ell \longrightarrow W_\ell \longrightarrow W_\ell{}^S \longrightarrow U_\ell{}^S \longrightarrow p^S$$

The Fermi case can be related to the Boltzmann case in the same way, with a convenient definition of the $W_\ell{}^A$ and $U_\ell{}^A$, and the program would be

$$U_\ell \longrightarrow W_\ell \longrightarrow W_\ell{}^A \longrightarrow U_\ell{}^A \longrightarrow p^A$$

The U_ℓ contain all dynamical features without involving statistics. For the computation of the U_ℓ we refer to the first papers quoted at the begining of this section:

Examples:

$$U_1 = W_1 = U_1{}^S = W_1{}^S \quad \text{from the definitions.}$$

In momentum representation:

$$\begin{aligned} \langle k'|U_1|k\rangle &= \langle k'|e^{-\beta k^2}|k\rangle \\ &= \delta_{kk'}\, e^{-\beta k^2} \end{aligned} \tag{13.21}$$

and in coordinate representation:

$$\begin{aligned} \langle x'|U_1|x\rangle &= (1/\Omega)\sum e^{-\beta k^2}\, e^{i\vec{k}.(\vec{x}-\vec{x}')} \\ &\xrightarrow[\Omega\to\infty]{} \lambda^{-3}\, e^{-\frac{|\vec{x}-\vec{x}'|^2}{4\beta}} \end{aligned} \tag{13.22}$$

where $\lambda = (4\pi\beta)^{\frac{1}{2}}$. This is a Gaussian distribution. For $\beta = 0$, the width of the distribution is zero, and as β increases it spreads out. One can think of it as a diffusion problem (keep in mind that $\beta = 0$ means $T = \infty$).

§14. Diagram representation of the grand partition function

a) Numbered Primary Diagrams

We want to express the U^S in terms of the U.

Recall that:

$$\left.\begin{array}{l} \langle 1'|W_1|\,1\rangle \;=\; \langle 1'|U_1|\,1\rangle \\ \langle 1'2'|W_2|1\;2\rangle = \langle 1'|U_1|1\rangle\langle 2'|U_1|2\rangle + \langle 1'2'|U_2|1\;2\rangle \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \end{array}\right\} \quad (14.1)$$

$$\langle 1'2\ldots\,\ell'|W_\ell{}^S|1\;2\;\ldots\ell\rangle = \sum_{P'} P'\,\langle 1'2'\ldots\,\ell'|W_\ell|1\;2\;\ldots\ell\rangle \quad (14.2)$$

and

$$\left.\begin{array}{l} \langle 1'|W_1{}^S|1\rangle \;=\; \langle 1'|U_1{}^S|1\rangle \\ \langle 1'2'|W_2{}^S|1\;2\rangle = \langle 1'|U_1{}^S|1\rangle\,\langle 2'|U_1{}^S|2\rangle + \langle 1'2'|U_2{}^S|1\;2\rangle \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \end{array}\right\} \quad (14.3)$$

Using (14.2) we can write:

$$\langle 1'2'|W_2{}^S|1\;2\rangle \;=\; \langle 1'|U_1|1\rangle\,\langle 2'|U_1|2\rangle \;+\; \langle 1'2'|U_2|1\;2\rangle$$
$$+\,\langle 2'|U_1|1\rangle\,\langle 1'|U_1|2\rangle \;+\; \langle 2'1'|U_2|\;1\;2\rangle$$

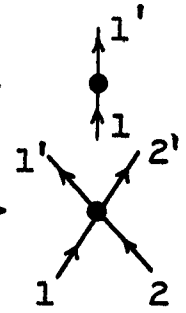
Comparing with (14.3), we conclude, as $\langle 1'|U_1|1\rangle = \langle 1'|U_1{}^S|1\rangle$, etc. that:

$$\langle 1'2'|U_2{}^S|1\;2\rangle = \langle 2'|U_1|1\rangle\,\langle 1'|U_1|2\rangle + \langle 1'2'|U_2|1\;2\rangle +$$
$$+\,\langle 2'1'|U_2|1\;2\rangle$$

In the same way the other U^S are found in terms of the U's. The computation is simplified by introducing a diagram representation e.g.:

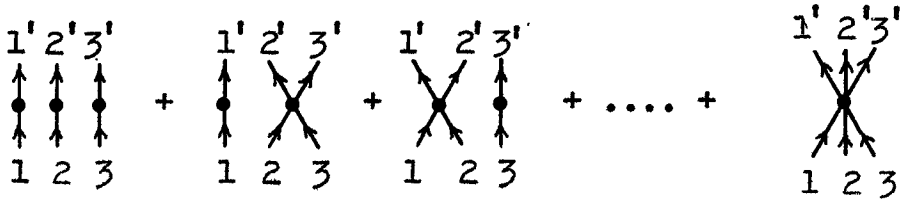
$\langle 1'|U_1|1\rangle \longleftrightarrow$

$\langle 1'2'|U_2|1\;2\rangle \longleftrightarrow$



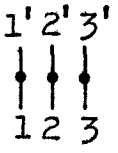
and so on.

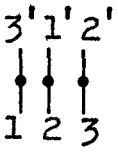
Then every W_ℓ is a sum of groups of such diagrams. For instance

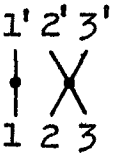
$W_3 =$ 

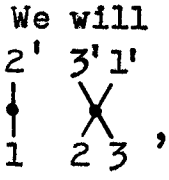
W_3^s contains all terms in W_3 plus the ones obtained by permutations of the primed numbers.

Comparing the W_3^s thus obtained with the corresponding expression as given by eq. (14.3), we obtain the graphical expression of U_3^s. The rule is to strike out from W_3^s all terms in which, when we make $1' = 1$, $2' = 2$, etc., the dependence on some of the coordinates is completely factored out. For simplicity we omit the arrows from now on.

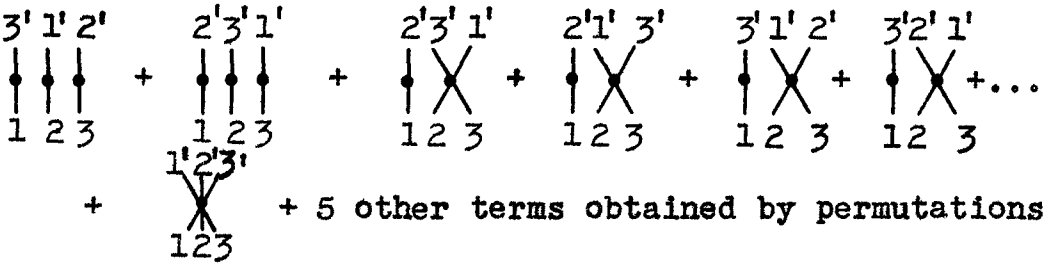
We will strike out 

but not 

; 

but not 

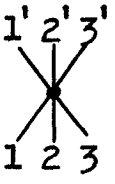
, etc. Then:

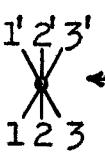
$U_3^s =$ 

+ 5 other terms obtained by permutations

Let us introduce

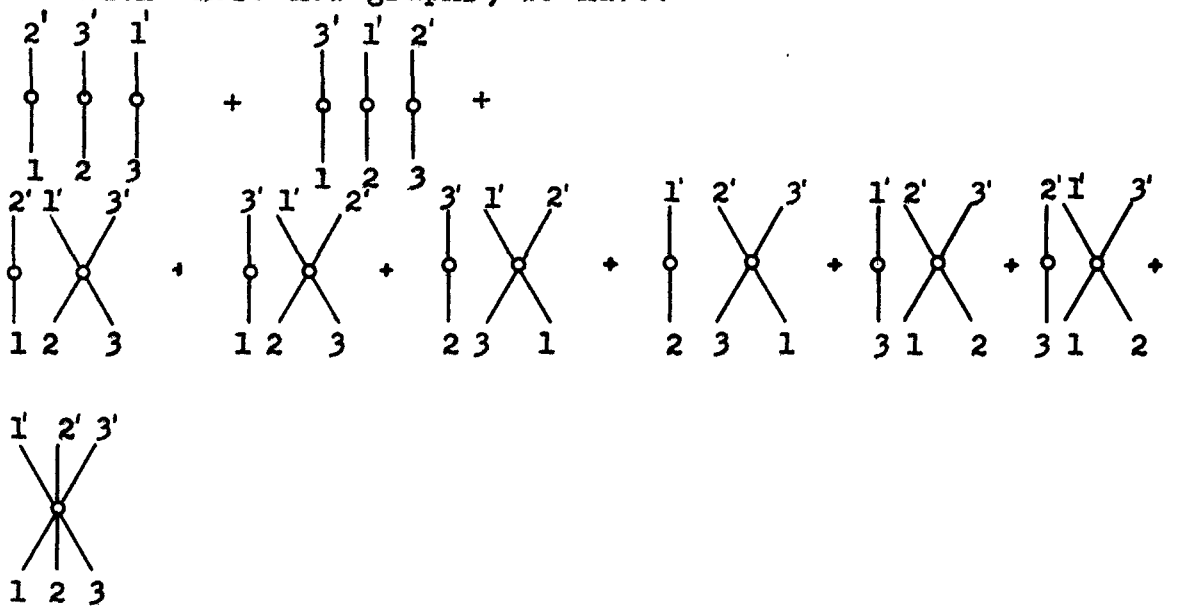
$$\langle 1'2'\ldots \ell' | \Upsilon_\ell | 1\ 2 \ldots \ell \rangle \equiv \sum_{P'} P' \langle 1'2'\ldots \ell' | U_\ell | 1\ 2 \ldots \ell \rangle \qquad (14.4)$$

e.g. 

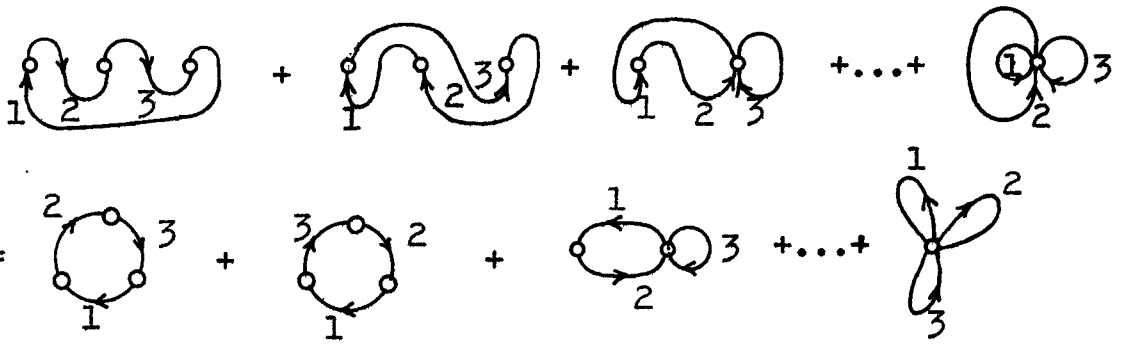
+ 5 others $= \langle 1'2'3' | \Upsilon | 1\ 2\ 3 \rangle \equiv$ 

← circle instead of point

With these new graphs, we have:

$U_3^S =$ 

As we are interested in the case $1' = 1$, $2' = 2$, ..., we indicate this by connecting lines with same indices:

$U_3^S =$ 

These are the <u>numbered primary diagrams</u>.

b) <u>Unnumbered primary diagrams</u>

As we are going to integrate over all coordinates, it is clear that several graphs give the same contributions, such as and . Since in the expression for $\ln Q^s$, we are summing over all diagrams, the total contribution of such

similar diagrams can be represented by a diagram without indices with an appropriate factor. These will be called the unnumbered primary diagrams. It can be proved that:

<u>Theorem</u>

$$\ln Q^S = \Sigma(\text{all unnumbered primary diagrams}) \qquad (14.5)$$

In the computations, an unnumbered primary diagram is defined to contain

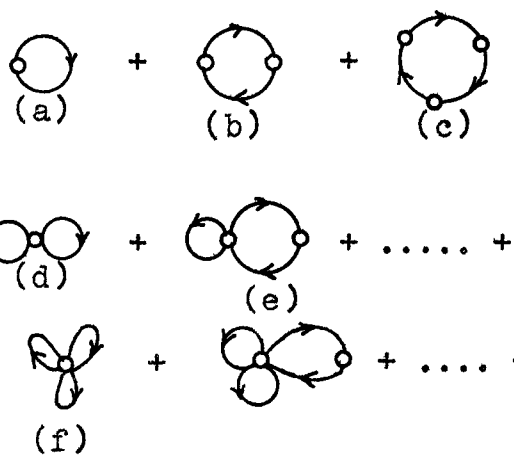
i) a factor z for each line; ℓ lines $\Rightarrow z^{\ell}$,

ii) a factor Υ for each junction,

iii) a factor 1/S where S is the symmetry number known from the theory of graphs).

S is the number of identical graphs within the totality obtained by all possible permutations of the indices in the original one.

To acquaint ourselves with the above statements, we write the first few diagram explicitly:

$\ln Q^S =$ 

(14.6)

$(a) \longrightarrow (Z/1)\int \langle 1|\Upsilon_1|1\rangle \, dl$

(b) $\longrightarrow (Z^2/2) \int \langle 2|T_1|1\rangle \langle 1|T_1|2\rangle \quad d1\ d2$

(c) $\longrightarrow (Z^3/3) \int \langle 2|T_1|1\rangle \langle 3|T_1|2\rangle \langle 1|T_1|3\rangle \quad d1\ d2\ d3$

(d) $\longrightarrow (Z^2/2) \int \langle 1\ 2\ |T_2|1\ 2\rangle \quad d1\ d2$

(e) $\longrightarrow (Z^3/1) \int \langle 2|T|3\rangle \langle 1\ 3|T_2|2\ 3\rangle \quad d1\ d2\ d3$

(f) $\longrightarrow (Z^3/6) \int \langle 1\ 2\ 3|T|1\ 2\ 3\rangle \quad d1\ d2\ d3$

c) <u>Contracted diagrams</u>

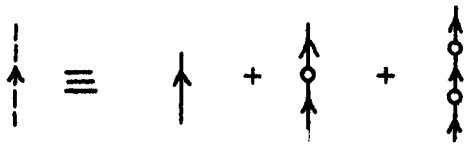
Since (cf. eq. (13.21)).

$$\langle k'\ |T|\ k\rangle = \delta_{kk'}\ e^{-\beta k^2} \tag{14.7}$$

it is simpler to carry out the computations in momentum space, and we shall do so. Consider (14.6): the contribution of the first row diagrams is:

$$\sum_k Z\ e^{-\beta k^2} + \sum_k (Z^2/2)\ e^{-2\beta k^2} + \sum_k (Z^3/3)\ e^{-3\beta k^2} + \ldots = \\ = -\ln\left(1 - Z\ e^{-\beta k^2}\right)$$

To represent more schematically the following rows of diagrams, we define:

$m(k) \equiv$  $+ \ldots =$

$$= Z + Z^2\ e^{-\beta k^2} + Z^3\ e^{-2\beta k^2} = \tag{14.8}$$

$$= Z/(1 - Z\ e^{-\beta k^2})$$

The motivation of this is that, for any given row, successive diagrams are obtained from the first just by interpolating

junctions Υ_1 in any of the lines. The set of diagrams of the second row is represented now by

;

the set of the third by

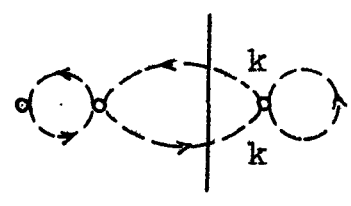
; and so on.

These are the <u>contracted diagrams</u>. To each of these is attached a symmetry factor, to be computed in the same way as before, now with respect to the dotted lines. It can be checked that the symmetry factor takes into account correctly the individual symmetry factors attached to the previous diagrams.

The introduction of the contracted diagrams is equivalent to having summed all Υ_1 terms, so that only the $\Upsilon_2, \Upsilon_3, \ldots$ remain.

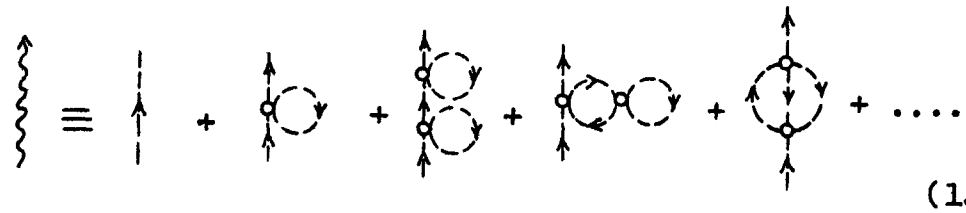
§15. Formulation in terms of average occupation numbers

The motivation of this is an extension of the previous development. Further sums can be performed. For instance, consider the following graph with the cut indicated:

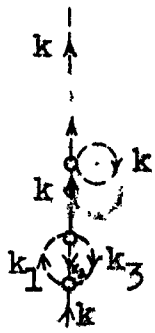


On the right of the cut, because of momentum conservation one has the same momentum on the two lines that cross the cut. This right side can be thought as a sort of a propagator.

We can sum over all such portions, i.e. portions which yield an outgoing momentum equal to the ingoing. To indicate this, we define:

$M(k) \equiv$  (15.1)

with the corresponding symmetry factor (same definition). Some example of contributions are (for the definition of m(k) see eq. (14.8)).



$$\rightarrow m(k)$$

$$\rightarrow m^2(k) \sum_{k'} \langle kk' | T_2 | kk' \rangle$$

$$\rightarrow \frac{1}{2} \sum_{k_1 k_2 k_3} m^2(k) \langle k_1 k_3 | T_2 | k k_2 \rangle \langle k k_2 | T_2 | k_1 k_3 \rangle \times \delta_{k+k_2-k_1-k_3}$$

It can be proved that M(k) has a direct physical meaning:

<u>Theorem</u>:

If $\langle n_k \rangle$ is the average occupation number in momentum state k in the grand canonical ensemble, then

$$\langle n_k \rangle = \sum_{\ell=1}^{\infty} (\ell Z^{\ell}/\ell!) \sum_{\substack{k_1 k_2 \ldots k_{\ell-1} \\ k \text{ fixed}}} \langle k\, k_1\, k_2 \ldots k_{\ell-1} | U_{\ell}^{S} | k\, k_1 \ldots k_{\ell-1} \rangle \tag{15.2}$$

Summing over k, both sides yield the total number of particles.

One can further prove the

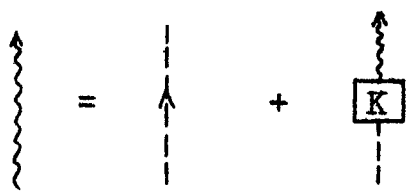
<u>Theorem</u>:

$$\langle n_k \rangle = M(k)/Z - 1 \tag{15.3}$$

where $Z = e^{-\beta\mu}$; μ: chemical potential.

<u>Steps to express $\ln Q^s$ in terms of M(k)</u>

(i)

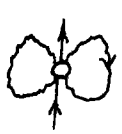


where

$K(k) =$ (15.4)

Explicitly:

$\longrightarrow \sum_{k'} \langle k\ k' | \Upsilon_2 | k\ k' \rangle\ M(k)$

 $\longrightarrow \frac{1}{2} \sum_{k_1 k_2} \langle k\ k_1 k_2 | \Upsilon_3 | k\ k_1\ k_2 \rangle\ M(k_1) M(k_2)$

which is only the summation of the proper part of the diagram.

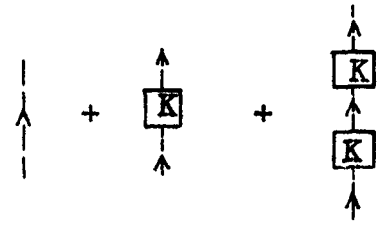
Then:

$$M = m + mKM \tag{15.5}$$

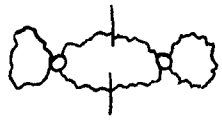
which gives the expansion

$$M = m + mKm + mKmKm +$$

+ all irreducible diagrams with lines

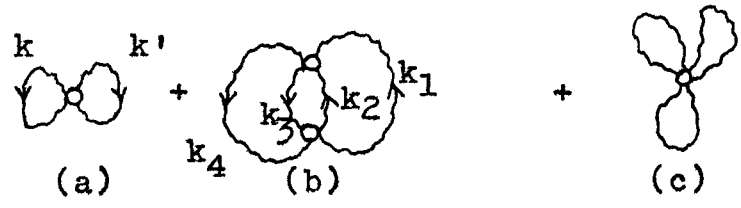
M =  + ... (15.6)

Irreducible diagrams: diagrams which, when two different lines are cut, do not split themselves into disconnected fragments.

 : this figure shows a reducible diagram.

(ii) Define

$\mathbb{P} = \Sigma$ (all irreducible diagrams with $\sim$ lines <u>without</u> external lines) =

= 

+ .... (15.7)

(a) $\rightarrow \frac{1}{2}\Sigma\langle k\ k'|\mathcal{T}_2|k\ k'\rangle\ M(k)\ M(k')$

(b) $\rightarrow (1/8)\Sigma\langle k_3\ k_4|\mathcal{T}_2|k_1\ k_2\rangle\ \langle k_1\ k_2|\mathcal{T}_2|k_3\ k_4\rangle$

$\times\ M(k_1)\ M(k_2)\ M(k_3)\ M(k_4)$

(c) $\rightarrow (1/6)\ \Sigma\ \langle 1\ 2\ 3|\mathcal{T}_3|1\ 2\ 3\rangle\ M(1)\ M(2)\ M(3)$

It can be proved the

<u>Lemma</u>

$$\frac{\delta\,\mathbb{P}}{\delta M(k)} = K(k) \tag{15.8}$$

<u>Theorem</u>

$$\ln Q^s = \Sigma\left[\ \ln\left[M(k)/Z\right] - M(k)/m(k) + 1\right] + \mathbb{P} \tag{15.9}$$

where

$$m(k) = Z/(1 - Z\, e^{-\beta k^2}) \tag{15.10}$$

and $\mathbb{P}$ is given by (15.7).

Main point for the proof of this theorem: if we differentiate both sides of the equation with respect to $\ln Z$, we obtain

$$\Sigma \langle n_k \rangle = \Sigma \left[M(k)/Z - 1\right]$$

which is clearly correct.

Use is made of eq. (15.6).

This theorem can be generalized into a variational principle:

<u>Theorem</u> (Variational Principle)

Consider

$$\mathcal{F} \equiv \Sigma \left\{ \ln[M(k)/Z] - M(k)/Z + M(k)e^{-\beta k^2} + 1 \right\} + \mathbb{P}$$

as a functional of M (for fixed Z). We seek the maximum of $\mathcal{F}$ with respect to variations of M.

$$\frac{\delta \mathcal{F}}{\delta M} = 1/M - 1/Z + e^{-\beta k^2} + K \tag{15.11}$$

where use is made of eq. (15.8).

Equating to zero, we get $M = m + m\,K\,M$. Therefore the grand partition function is a stationnary value of $\mathcal{F}$. It can be proved that it is in fact a maximum by taking the second variation.

In this way the thermodynamical problem is formulated in

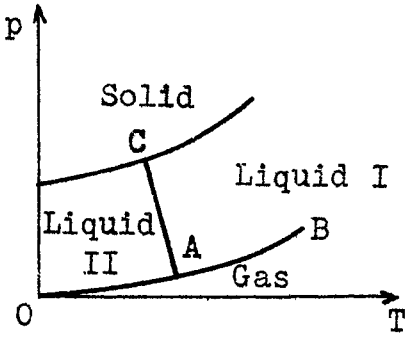
terms of a variational principle.

§16. Comparison with the physical situation

The grand partition function is expressed in terms of M, Z and $\mathbb{P}$ (eq. (15.9)). $\mathbb{P}$, as given by eq. (15.7), involves the Υ functions which contain no statistics: it depends only on the dynamics of the system.

For certain T and Z, M(k) has singularities in its dependence on k, i.e. at k = 0 $M \longrightarrow \infty$. Bose-Einstein transition obtains when the variational principle leads to a M(k) that becomes singular at k = 0.

For the real He^4 system the phase diagram is as illustrated.



The results above lead to the expectation that

Along AB M(k) = finite on both sides

Along AC M(0) = infinite on both sides

Along OA M(0) $\begin{cases} = \text{infinite on liquid side} \\ = \text{finite on gas side} \end{cases}$

.:.:.:.:.:.:.:.:.