JUN 2 1963

Lab 5813
MASTER 79179

The Ground State Energy and Sound Velocity of a System of Interacting Bosons

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ABSTRACT

The Method of Padé approximants is used to evaluate the ground state energy, E_0 , of a system of interacting Bosons. The density, ρ_0 , of particles in the zero momentum state appears as a free parameter. In particular, the method is applied to a system of hard spheres of radius c and density ρ . The result is close to the exact value for low densities and has a singularity at a density which corresponds to close packing when $\rho_0 = \rho/4$. The calculated sound velocity as a function of ρ coincides with the experimental values for liquid helium II for $\rho_0 = \frac{1}{2} \rho$ and $c = 2.16 \text{ \AA}$.

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I. Introduction

The object of this paper is to describe a method of calculating the properties of a system of Bosons which may be applicable to liquid helium II.

One approach to this problem is to sum selected terms in perturbation theory¹ and, in this way it is not too difficult to deal with a weakly interacting system at very high density or a strongly interacting system at very low density — provided the inter-particle forces are repulsive. In liquid helium, the forces are strong and partly attractive and the density is neither very high nor very low. If the attractive part of the force were neglected, a combination of the high and low density theories could be attempted,¹ but it would be exceedingly difficult to justify the omission of intermediate density terms.

Consequently, although this approach has provided a physical picture of the behaviour of liquid helium it needs further modification to produce numerical results in agreement with experiment.²

In the method to be described here, all terms of a given order of perturbation theory are included and a sequence of Padé approximants³ is constructed to simulate the behaviour of the complete perturbation series. For example, if the ground state energy per particle E_0 , is calculated as a power series

¹ K. A. Brueckner and K. Sawada, Phys. Rev., 106, 1117, 1128 (1957).

² W. E. Parry and D. ter Haar, Ann. Phys., 19, 496 (1962).

³ H. S. Wall, Continued Fractions (D. Van Nostrand Co., Inc., Princeton, 1948).

in the strength, V_0 , of the interaction between the particles,

$$E_0 = \sum_{p=0}^{\infty} E_p V_0^p \quad (1)$$

then the (n,m) Padé approximant $P_m^n(V_0)$ is defined as

$$P_m^n(V_0) = \frac{a_0 + a_1 V_0 + a_2 V_0^2 + \dots + a_n V_0^n}{1 + b_1 V_0 + b_2 V_0^2 + \dots + b_m V_0^m} \quad (2)$$

where the a_i and b_j are chosen so that if $P_m^n(V_0)$ is expanded as a power series in V_0 , the first $(m+n)$ terms coincide with the first $(m+n)$ terms in the expansion of E_0 . This prescription defines the a_i and b_j uniquely. When expanded, $P_m^n(V_0)$ contains all powers of V_0 and so gives an approximation to the complete perturbation series which may be useful for very large values of V_0 . In particular, P_m^n has a finite limit a_n/b_n as $V_0 \rightarrow \infty$ so that a hard core interaction may be dealt with in this way.

Usually, the evaluation of successive terms in a many-body perturbation series is very laborious, but, for an infinite system of Bosons, the unperturbed state is extremely simple — every particle has zero momentum — and it is not too difficult to calculate the first few orders in the expansion of the ground state energy and so to explore the potentialities of the approach before proceeding to discuss other properties and other systems.

In Section II the ground state energy is evaluated to fourth order in perturbation theory and the removal of the divergences characteristic of the many-Boson problem is discussed. To this order, it is necessary to introduce an adjustable parameter which is identified with the density, ρ_0 , of particles

in the zero momentum state. The expressions are evaluated in particular for a finite repulsive core interaction of height V_0 and radius c . In Section III, the Padé approximants P_1^1 and P_2^2 are evaluated in the limit $V_0 \rightarrow \infty$ to give an estimate of the ground state energy of a set of hard sphere Bosons as a function of their density ρ . $P_2^2(\infty)$ is close to the exact value $(2\pi\rho c)$ at low densities and also shows a singularity at a density which may be made to correspond to close packing by choice of ρ_0 . The velocity of sound, u , calculated from this approximation as a function of ρ coincides with the experimental values for liquid helium II if ρ_0 is $\frac{1}{2}\rho$ and c is 2.16 Å. The rise in u as ρ increases is a consequence of the approach to the close packing singularity.

II. The Perturbation Series for the Ground State Energy

The Hamiltonian H for the system may be separated into unperturbed part H_0 and perturbation V so that

$$H = H_0 + V \quad (3)$$

and, in second quantization notation,

$$H_0 = \sum_{\underline{k}} \frac{1}{2} k^2 a_{\underline{k}}^* a_{\underline{k}} \quad (4)$$

$$V = \frac{1}{2\Omega} \sum_{\underline{k}, \underline{q}, \underline{q}'} v(\underline{q} - \underline{q}') a_{\frac{1}{2}\underline{k}+\underline{q}}^* a_{\frac{1}{2}\underline{k}-\underline{q}}^* a_{\frac{1}{2}\underline{k}+\underline{q}} a_{\frac{1}{2}\underline{k}-\underline{q}} \quad (5)$$

Here, units have been chosen so that $\hbar = 1$, $m = 1$ and Ω is the normalization volume. The operators $a_{\underline{k}}^*, a_{\underline{k}}$ respectively create and annihilate a particle of momentum $\underline{k}$ and satisfy the commutation relations

$$[a_{\underline{k}}, a_{\underline{k}'}] = 0 = [a_{\underline{k}}^*, a_{\underline{k}'}^*] \quad (6)$$

$$[a_{\underline{k}}, a_{\underline{k}'}^*] = \delta_{\underline{k} \underline{k}'} \quad (7)$$

If the potential energy of a pair of particles of separation r is given by $v'(\underline{r})$ then

$$v(\underline{k}) = \int d\underline{r} v'(\underline{r}) e^{-i\underline{k} \cdot \underline{r}} \quad (8)$$

The ground state of the unperturbed Hamiltonian is obtained by putting every particle in the plane wave state of zero momentum and it is this fact which makes the problem reasonably tractable.

Many-body perturbation theory and its application to a Bose gas has been reviewed in some detail by Brueckner⁴ and the details will not be repeated here.

The characteristic feature of the perturbation theory of a Bose gas is that beyond second order, there occur terms which diverge in the limit of infinite volume as a consequence of the dominant role played by the zero momentum state. One of the objects of the method introduced by Brueckner and Sawada¹ is to remove this divergence by a partial summation of terms from all orders of perturbation theory.

If the divergent parts are separated out in each order then the first four terms of the perturbation series are

$$\Delta E_1 = \frac{1}{2} \rho v(0) \quad (9)$$

$$\Delta E_2 = \frac{1}{2} \frac{\rho}{\Omega} \sum_{\vec{q} \neq 0} \frac{v^2(\vec{q})}{q^2} \quad (10)$$

$$\Delta E_3 = \Delta E_3(1) + \Delta E_3(2) + \Delta E_3^D(0) \quad (11)$$

$$\Delta E_4 = \Delta E_4(1) + \Delta E_4(2) + \Delta E_4(3) + \Delta E_4(4) + \Delta E_4(5) + \Delta E_4^D(0) \quad (12)$$

where ρ is the number density and

$$\Delta E_3(1) = \frac{\rho}{\Omega^2} \sum_{\vec{q}_1 \neq 0} \sum_{\vec{q}_2 \neq 0} v(\vec{q}_1) \frac{1}{q_1} v(\vec{q}_1 - \vec{q}_2) \frac{1}{q_2} v(\vec{q}_2) \quad (13)$$

$$\Delta E_3(2) = \frac{\rho^2}{\Omega} \sum_{\vec{q} \neq 0} \frac{v^3(\vec{q}) - v^3(0)}{q^4} \quad (14)$$

⁴ Dewitt (ed.), The Many Body Problem (Dunod, Paris 1959).

$$\Delta E_4(1) = -\frac{1}{2} \frac{\rho}{\Omega^3} \sum_{\underline{q}_1 \neq 0} \sum_{\underline{q}_2 \neq 0} \sum_{\underline{q}_3 \neq 0} \frac{v(\underline{q}_1) v(\underline{q}_1 - \underline{q}_2) v(\underline{q}_2 - \underline{q}_3) v(\underline{q}_3)}{q_1^2 q_2^2 q_3^2} \quad (15)$$

$$\Delta E_4(2) = -\frac{3\rho^2}{\Omega^2} \sum_{\underline{q}_1 \neq 0} \sum_{\underline{q}_2 \neq 0} \frac{v(\underline{q}_1) v(\underline{q}_1 - \underline{q}_2)}{q_1^2} \left[\frac{v^2(\underline{q}_2) - v^2(0)}{q_2^4} \right] \quad (16)$$

$$\Delta E_4(3) = -\frac{\rho^2}{\Omega^2} \sum_{\underline{q}_1 \neq 0} \sum_{\underline{q}_2 \neq 0} \left\{ v^2(\underline{q}_1) v(\underline{q}_2) \left[v(\underline{q}_2) + v(\underline{q}_2 - \underline{q}_1) \right] - \frac{2v^4(0) q_0^2}{q_1^2 q_2^2 + q_0^2} \right\} \quad (17)$$

$$\times \frac{1}{q_1^4} \left\{ \frac{q_1^2 + q_2^2 + (\underline{q}_1 - \underline{q}_2)^2}{q_1^2 + q_2^2 + (\underline{q}_1 - \underline{q}_2)^2} - \frac{1}{q_2^2} \right\}$$

$$\Delta E_4(4) = -\frac{2\rho^2}{\Omega^2} \sum_{\underline{q}_1 \neq 0} \sum_{\underline{q}_2 \neq 0} \left\{ \frac{v(\underline{q}_1) v(\underline{q}_2) [v(\underline{q}_1 - \underline{q}_2) + v(\underline{q}_1)] [v(\underline{q}_2 + v(\underline{q}_1 - \underline{q}_2))]}{q_1^2 q_2^2 [q_1^2 + q_2^2 + (\underline{q}_1 - \underline{q}_2)^2]} \right. \quad (18)$$

$$\left. - \frac{4 v^4(0) q_0^2}{q_1^2 + q_2^2 + q_0^2} \frac{1}{q_1^2 q_2^2 [q_1^2 + q_2^2 + (\underline{q}_1 - \underline{q}_2)^2]} \right\}$$

$$\Delta E_4(5) = -5/2 \frac{\rho^3}{\Omega} \sum_{\underline{q} \neq 0} \frac{v^4(\underline{q}) - v^4(0)}{q^6} \quad (19)$$

$$\Delta E_3^D(\epsilon) = \frac{\rho^2}{\Omega} \sum_{\underline{q} \neq 0} \frac{v^3(0)}{(q^2 + \epsilon^2)^2} \quad (20)$$

$$\Delta E_4^D(\epsilon) = \frac{-3\rho^2}{\Omega^2} \sum_{\tilde{q}_1 \neq 0} \sum_{\tilde{q}_2 \neq 0} \frac{v(\tilde{q}_1) v(\tilde{q}_1 - \tilde{q}_2) v^2(0)}{q_1^2 (q_2^2 + \epsilon^2)^2}$$

$$- \frac{2\rho^2}{\Omega^2} \sum_{\tilde{q}_1 \neq 0} \sum_{\tilde{q}_2 \neq 0} \frac{v^4(0) q_0^2}{q_1^2 + q_2^2 + q_0^2} \frac{1}{(q_1^2 + \epsilon^2)^2} \left\{ \frac{2}{q_1^2 + q_2^2 + (q_1 - q_2)^2 + \epsilon^2} - \frac{1}{q_2^2 + \epsilon^2} \right\}$$
(21)

$$- \frac{8\rho^2}{\Omega^2} \sum_{\tilde{q}_1 \neq 0} \sum_{\tilde{q}_2 \neq 0} \frac{v^4(0) q_0^2}{q_1^2 + q_2^2 + q_0^2} \frac{1}{(q_1^2 + \epsilon^2)(q_2^2 + \epsilon^2) [q_1^2 + q_2^2 + (q_1 - q_2)^2 + \epsilon^2]}$$

$$- \frac{5}{2} \frac{\rho^3}{\Omega} \sum_{\tilde{q} \neq 0} \frac{v^4(0)}{(q^2 + \epsilon^2)^6}$$

ΔE_3 and ΔE_4 have been rearranged in this way so that $\Delta E_3^D(0)$ and $\Delta E_4^D(0)$ are the only terms which diverge in the limit of infinite volume. The quantity $q_0^2(q_1^2 + q_2^2 + q_0^2)$ has been included to ensure convergence of the sums for high momenta. Since it replaces $v(q)$ in this role, q_0 should be of the order of the reciprocal of the range of $v(r)$.

One method of dealing with the divergences would be to replace $\Delta E_3^D(0)$ and $\Delta E_4^D(0)$ by $\Delta E_3^D(\epsilon)$ and $\Delta E_4^D(\epsilon)$ respectively in Eqs. (11) and (12), then to form the Padé approximants and finally to let ϵ tend to zero. However, in order to obtain a significant result from this procedure, it is necessary to work to a much higher order in perturbation theory.

Consequently it is better to adopt the alternative approach of summing selected terms from the divergent parts of higher orders of perturbation theory so as to leave a finite value of ϵ in the energy denominators. This procedure has been carried out by Brueckner and Sawada¹ who show that for $\Delta E_3^D(\epsilon)$ and the ρ^3 term of $\Delta E_4^D(\epsilon)$, a first approximation for ϵ is given by

$$\epsilon^2 = 8\pi \rho_0 \underline{a}$$
(22)

where ρ_0 is the density of particles in the zero momentum state² and $\underline{a}$ is the scattering length of the interaction. The value of ϵ which should be used in the ρ^2 terms of $\Delta E_4^D(\epsilon)$ is not given by Eq. (22) but the difference should not be too large and it will be neglected. In this approach, there is no prescription for calculating ρ_0 and it will be treated as a free parameter. If $\underline{a} < 0$, Eq. (22) cannot be used and ϵ must be treated as a free parameter.

The scattering length, $\underline{a}$, may be expressed as a power series in the coupling constant so if Eq. (22) is used to define ϵ and $\Delta E_3^D(\epsilon)$ is expanded in powers of the coupling constant, there will be a fourth order contribution which should be subtracted from $\Delta E_4^D(\epsilon)$. To lowest order, ρ_0 may be replaced by ρ and the result is that the factor $(-5/2)$ in the ρ^3 term of $\Delta E_4^D(\epsilon)$ has to be replaced by $(3/2)$.

The simplest case of some physical interest is a system of hard spheres, whose behaviour is well understood at very high and very low densities. The potential, $v'(r)$, is given by

$$v'(r) = \begin{cases} V_0 & \text{for } r \leq c \\ 0 & \text{for } r > c \end{cases} \quad (23)$$

and after the formation of the Padé approximants, V_0 will be allowed to become infinite. For finite V_0 , the scattering length is given by

$$a = c - \frac{\tanh V_0^{\frac{1}{2}} c}{V_0^{\frac{1}{2}}} \quad (24)$$

which becomes equal to c when $V_0 \rightarrow \infty$. q_0 is to be set equal to c^{-1} .

In the limit of infinite volume, the sums in Eqs. (9) to (21) become integrals of which only $\Delta E_4(3)$, $\Delta E_4(4)$ and those which contain q_0 in $\Delta E_4^D(\epsilon)$ have to be evaluated numerically. In particular ΔE_1 , ΔE_2 , $\Delta E_3(1)$ and $\Delta E_4(1)$ are the first four terms in the expansion of $2\pi\rho a$ and can be determined by expanding the right-hand side of Eq. (24) in powers of V_0 .

The results are

$$E_1 = \Delta E_1 V_0^{-1} = \frac{2\pi}{3} \rho c^3 \quad (25)$$

$$E_2 = \Delta E_2 V_0^{-2} = \frac{-4\pi}{15} \rho c^5 \quad (26)$$

$$E_3 = \Delta E_3 V_0^{-3} = \frac{34\pi}{315} \rho c^7 - \frac{6231 \pi^2}{16800} \rho^2 c^{10} + \frac{8 \pi^2}{27} \frac{\rho^2 c^9}{\epsilon} \quad (27)$$

$$\begin{aligned} E_4 = \Delta E_4 V_0^{-4} = & -\frac{124\pi}{2835} \rho c^9 + 3.064 \rho^2 c^{12} - 11.34 \rho^3 c^{15} \\ & - \frac{16\pi^2}{45} \frac{\rho^2 c^{11}}{\epsilon} + \frac{8\pi^3}{27} \frac{\rho^3 c^{14}}{\epsilon} - \frac{20\pi^3}{81} \frac{\rho^3 c^{12}}{\epsilon^3} \\ & - I(\epsilon) \end{aligned} \quad (28)$$

$I(\epsilon)$ has to be found numerically for each value of ϵ . For small values of ϵ ,

$$I(\epsilon) \approx \left[\left(\frac{\sqrt{3}}{4} \pi - \frac{\pi^2}{3} \right) \log \epsilon^2 c^2 - 5.566 \right] \frac{64}{81} \rho^2 c^{12} \quad (29)$$

III. Padé Approximation

The first diagonal Padé approximant $P_1^1(V_0)$ of the perturbation series for the energy is given by

$$P_1^1(V_0) = \frac{2\pi}{3} \rho c^3 \frac{V_0}{1 + 2/5 c^2 V_0} \quad (30)$$

$$\rightarrow 5/6 (2\pi\rho c) \quad (31)$$

as $V_0 \rightarrow \infty$. This result may be compared with the low density limit of $2\pi\rho c$ obtained by Lee, Huang and Yang.⁵ It is clearly inadequate at all but the lowest densities.

The second Padé approximant $P_2^2(V_0)$ has the form

$$P_2^2(V_0) = \frac{a_0 + a_1 V_0 + a_2 V_0^2}{1 + b_1 V_0 + b_2 V_0^2} \quad (32)$$

The method of calculating the a_i and b_j from E_1, E_2, E_3 and E_4 is described in Section I and it is found that

$$\lim_{V_0 \rightarrow \infty} P_2^2(V_0) = a_2/b_2 = \frac{2E_1 E_2 E_3 - E_2^3 - E_1^2 E_4}{E_2 E_4 - E_3^2} \quad (33)$$

which may be evaluated with the aid of Eqs. (25) to (28) and Eq. (22). The numerator and denominator of the result may each be reduced to the sum of a polynomial of fourth degree in $\sqrt{\rho c^3}$ and a term depending upon $\log \rho c^3$. The coefficients depend upon ρ_0 .

In Fig. 1, $P_2^2(\infty)$ is shown as a function of $(\rho c^3)^{-1}$ for several values of ρ_0 .

⁵ T. D. Lee, K. Huang and C. N. Yang, Phys. Rev., 106, 1135 (1957).

It has a quite different behaviour from $P_1^1(\infty)$. The discussion of Fig. 1 will be separated into three parts.

(a) Low Densities

Here $\rho_0 \rightarrow \rho$ and

$$P_2^2(\infty) = 2\pi\rho c \left\{ \frac{14}{15} \frac{1 + 1110.3 \sqrt{\rho c^3} + \dots}{1 + 1208.5 \sqrt{\rho c^3} + \dots} \right\} \quad (34)$$

Clearly, there is no point in expanding this expression in powers of $\sqrt{\rho c^3}$ and the second term of the expansion would not coincide with the exact expression.⁵ However the numerical value is close to the low density limit of $2\pi\rho c$. The very large coefficients of $\sqrt{\rho c^3}$ occur because both numerator and denominator had to be multiplied by large factors to make their leading terms unity. This feature is a consequence of the fact that the coefficients a_2 and b_2 in the P_2^2 approximant of the expansion of a in Eq. (24) are very small.

(B) High Densities

E_0 should have a double pole⁶ at the close packing density

$$\rho c^3 = \sqrt{2} \quad (35)$$

As can be seen from Fig. 1, P_2^2 has a singularity but it is a simple pole. Of course, at close packing, a given particle interacts strongly with twelve other particles so that an approximation based upon fourth order perturbation theory and thus including no more than four body collisions with any accuracy would not be expected to be valid. Nevertheless for $\rho_0 = 1/4 \rho$, the singularity in P_2^2 occurs at the density given by Eq. (35).

⁶F. London, Superfluids, Volume II (John Wiley & Sons, Inc., New York, 1954).

Higher Padé approximants are unlikely to introduce a double pole but may have a second pole at a density somewhat higher than that for close packing.

(c) Liquid Helium Densities

On the basis of the Keesom - Taconis⁷ model of liquid helium one may estimate crudely that a given helium atom interacts simultaneously with about six others, although the structure is considerably less rigid than that of a close packed crystal. Consequently P_3^3 could be a good approximation at liquid helium densities and P_2^2 may not be too inaccurate.

One quantity which may be calculated for a system of hard spheres and compared with experiments on liquid helium is the sound velocity u given by

$$u^2 = \frac{d}{d\rho} \left(\rho^2 \frac{dE_0}{d\rho} \right) \quad (36)$$

c is to be interpreted as an effective hard core radius which should be rather less than the radius, 2.56 Å, of the repulsive part of the interaction between helium atoms. The calculation may be regarded as an attempt to estimate ρ_0 and c for liquid helium by choosing them to fit the experimental values of u as a function of ρ .

If the pressure of liquid helium is varied from the vapour pressure to 25 Atmospheres, the density increases by about 15% and, at 1.25°K, the sound velocity⁸ increases from 237 metres/sec to 365 metres/sec. From Eq. (36) it follows that this increase in the value of u may be attributed to the rise in E_0 as close packing density is approached. Since ρ varies by such a small amount, it is most reasonable to choose ρ_0 and c to fit the mean experimental values of u and $\frac{du}{d\rho}$. For $c = 2.16$ Å and $\rho_0 = \frac{1}{2}\rho$,

⁷ W. H. Keesom and K. W. Taconis, Physica 4, 28, 256 (1937); 5, 270 (1938).

the calculated and measured values of u agree to within a few percent. These values of ρ_0 and c are close to those estimated by Parry and ter Haar² on the basis of the theory of Brueckner and Sawada.¹

IV. Conclusions

The Padé approximant P_2^2 gives a good qualitative representation of E_0 for all densities and by choice of very plausible values of ρ_0 can be made to give quite accurate numerical results. To estimate the accuracy of the approximation within the framework of the method itself, it would be necessary to go to sixth order perturbation theory in order to compare P_3^3 with P_2^2 .

However, the results from fourth order perturbation theory are sufficiently encouraging to suggest that it would be worthwhile to calculate the energy spectrum in the same way and to introduce the true interaction between helium atoms.

V. Acknowledgments

Part of this work was carried out whilst two of the authors (V.J.E. and J.L.G.) were visitors in the Theoretical Physics Division at A.E.R.E. Harwell, England and they wish to acknowledge the hospitality of Dr. W. Marshall.

Figure Caption

Fig. 1: The second diagonal Padé approximation $P_2^2(\infty)$ to the energy divided by the exact low density limit $2\pi\rho\cdot\rho_0$ is the density of particles in the zero momentum state and, for liquid helium II $(\rho c^3)^{-\frac{1}{3}}$ is about 1.6.

$$\frac{M}{\hbar^2} \frac{E c^2}{2\pi\rho c}$$

4

3

2

1

0

1

2

3

4

5

$$(\rho c^3)^{-\frac{1}{3}}$$

1 $\rho_0 = \rho$

2 $\rho_0 = \frac{1}{2}\rho$

3 $\rho_0 = \frac{1}{4}\rho$

1

2

3