THE STRUCTURE OF THE NEGATIVE ION IN LIQUID HELIUM.

A Thesis presented by
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to the
University of St. Andrews
in application for the Degree of
Doctor of Philosophy.

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DECLARATION.

I hereby declare that the accompanying Thesis is my own composition, that it is based upon research carried out by me, and that no part of it has previously been presented in application for a Higher Degree.

CERTIFICATE

I certify that Roger Corthan Clark, B.A., has spent nine terms as a research student in the Department of Theoretical Physics of the United College of St. Salvator and St. Leonard in the University of St. Andrews; that he has fulfilled the conditions of the University Court Ordinance LXXIX (St. Andrews No. 16) and the supplementary Senate Regulations; and that he is qualified to submit the following Thesis in application for the Degree of Doctor of Philosophy.

Research Supervisor

CAREER.

In 1960, I graduated from the University of Oxford with a first class honours degree in Mathematics. After spending one year at the Clarendon Laboratory on a post-graduate course in Theoretical Physics, I was admitted by the Senatus Academicus of St. Andrews University as a Research Student. I received financial support from the Department of Scientific and Industrial Research during the year in Oxford and for the first two years of my research in St. Andrews. Since 1963, I have held the post of Assistant in the Department of Theoretical Physics in the University of St. Andrews and was appointed Lecturer in October 1965.

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Finally my gratitude is given to my wife who not only typed this thesis but without whose initial encouragement I might never have undertaken this research at all.

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CHAPTER 1.

INTRODUCTION.

1. The Problem.

A rigorous treatment of the motion of an electron in liquid helium would involve the elucidation of a complicated many-body problem. An electrons interaction with a helium atom is in itself a complex phenomenon that involves both electromagnetic forces and quantum mechanical effects. The problem of liquid helium alone is one that has drawn much attention and still has not been solved without many restrictions on the region of validity of the solution. The mathematical approach to any physical situation involves an idealization of it. In building a model we are forced to make fairly drastic assumptions that have to be justified and this may only be possible if we limit the ranges of the physical parameters that describe the problem. In this thesis we have tried to point to the approximations we have made and to justify them.

We would have liked to lift all restrictions on the theory but this was clearly impossible. Not only have we been forced to ignore the detailed structure of the helium atoms, to idealize their interactions but virtually to ignore the composition of the liquid altogether. We have had to judge which aspects of the problem could be covered by a blanketing parameter. For example, since we will only be considering low energy collisions between the electron and helium atoms, we have been able to conceal the profusion of forces that govern the scattering in the concept of a scattering-length. This has been justified both theoretically and by experiment for it has been shown that the low-energy scattering process is insensitive to the details of the collision.

The use of a purely repulsive interaction in place of the real helium atom-atom interaction is not so simply vindicated. Here we have had to appeal to mathematical expediency to excuse our model. The idea that the attractive part of the atom-atom potential may be described by a uniform external pressure is not valid for this problem and in this aspect our treatment is not realistic. This will be more quantitatively discussed in Chapter 3. when the Hamiltonian governing the motion of the electron is set up.

The problem we are studying is an interesting one. In 1959, Careri. Scaramuzzi and Thompson proposed that the negative ion in liquid helium might not only be an unbound electron but that this electron might be self-trapped in a cavity created by virtue of its high zero-point energy in the space between the helium atoms. The electron reduces this energy by repelling the helium atoms in its immediate vicinity. In 1960, Careri, Fasoli and Gaeta reported the results of some experiments that tested and confirmed this idea and pointed out that Ferrell (1957) had proposed independently a similar structure for the positronium atom in liquid helium. Kuper (1961) was the first to present a calculation of the size of the cavity based on sound physical arguments. He pointed out that the growth of the bubble was not restricted by surface tension as Ferrell had proposed nor by electrostriction (i.e. polarization of the atoms around the electron) but largely by the zero-point pressure exerted by helium atoms on the bubble. Kuper found that the radius of the bubble to be about twelve Angstroms, which leads to values of the effective mass and scattering cross-section that account remarkably well for the observed mobility. Kuper's estimate is still the touchstone against which other calculations are measured,

The idea of self-trapped electrons was originally put forward in 1933 by Landau to explain F-centers in ionic crystals. This early theory has grown into the well developed polaron problem considered by a number of authors (Fröhlich 1952, Landau and Pekar 1946, Tiablikov 1952, Feynman 1955 and others). The polaron problem has a number of points akin to the subject of this thesis, and many more if we extend the discussion to cover all impurities in liquid helium. This similarity has been pointed out by many physicists working on liquid helium problems, notably Gross (1958), Girardeau (1961) and Miller, Pines and Nozieres (1962). In this thesis we use as our starting point some ideas put forward by Gross (1958) and show that these lead to a bubble structure around a light particle, provided only that the interaction between the liquid helium and the particle is sufficiently strong.

2. Outline of the Thesis.

In the next chapter, we will look at Kuper's model of the negative ion and compare it with the band-like mode of propagation of an electron in liquid helium. We will also discuss the experimental evidence in favour of the bubble model and Atkins model of the positive ion to illustrate the effect of electrostriction. In Chapter 3. we will derive Gross' equations and, using a pseudo-potential to describe the interactions, express them in a form from which a bubble-like solution can be shown to exist. Chapter 3. also describes some computer calculations of these solutions showing clearly the extent of the cavity. In Chapter 4. we use a variational principal to obtain estimates of the energy of the bubble structure. The wave-functions which minimize the energy are compared with the computed ones. Also included in this chapter is a prediction of the existence of excited electronic states in the bubble and an estimate is made of the minimum coupling strength needed before a bubble state can be sustained.

Chapter 5. discusses how excited states of the bosons might be included in treatments of the problem and estimates their effect. The effective mass of the ion is shown to be determined by the bubble radius and that distortions of the bubble at low velocities are unimportant.

In Chapter 6. we consider the application of standard polaron techniques to the problem of an impurity of arbitrary mass in liquid helium. In particular it is shown that Feynman's path integral treatment seems to break down for this problem for any other trial action functional than a simple perturbation theoretic one. Chapter 7. shows that the bubble structure is not limited to boson systems but is rather the result of the relative energies of the impurity and the atoms of the surrounding liquid. An illustrative calculation for a fermion system is made. Finally in Chapter 8. conclusions and further problems are presented.

3. Notation.

Mostly a symbol is defined only when it is first used but occasionally, for clarity, its definition has been repeated. The convention $\hbar = \mu = 1$, where $\hbar$ is Plancks constant divided by 2π and μ is the impurity mass, has been used frequently but usually the reader is warned in the text when this occurs. The symbol μ stands for a general impurity mass, but sometimes more specifically for the electronic mass, $9{\cdot}1 \times 10^{-28}$ gms .

CHAPTER 2.

MODELS OF THE IONS IN He II.

In this chapter, we shall critically review the various models proposed for the ions in liquid He^4. The experimental evidence in favour of the bubble model will be presented as will be the theory of the band-like mode of propagation of the electron. The electron helium-atom scattering length will be discussed.

1. The Negative Ion.

The bubble model for the negative ion has been analyzed semi-phenomenologically by Kuper (1961). It is assumed that the negative ion is a free electron whose interactions with the atoms of the liquid are mainly short range repulsions. If the electron is localised in a sphere radius b_- , then the pressures exerted by the electron outward on the liquid have to be balanced by the inward pressures of the atoms on bubble. This leads to the equation

$$P_{kin} - P_{es} = E_0 \rho_0 + P_{vdW} \qquad (2\text{-}1)$$

where ρ_0 is the unperturbed number density and P_{kin} is the pressure due to the kinetic energy of the localised electron. P_{es} is the pressure due to the electrostatic forces between the electron and the polarized atoms. $E_0 \rho_0$ is the kinetic energy per unit volume of the atoms and P_{vdW} is the pressure term due to the van der Waals forces between the atoms. If the electron is taken as a particle in an infinitely deep spherical well, then $P_{kin} = \pi \hbar^2 / 4\mu b_-^5$ and the polarization term $P_{es} = \rho_0 e^2 \alpha / 2 b_-^4$ where α is the atomic polarizability. The van der Waals pressure may be calculated if we know the radial distribution function $g(|\underline{r}_i - \underline{r}_j|)$ of the atoms in the liquid. Kuper assumes that $g(r) = 0$ if $r < c$ where c is the mean interatomic distance in the liquid and $g(r) = \rho_0$ if $r > c$, and finds after a straightforward calculation that

$$P_{vdW} = -\left(\frac{3}{4\pi}\right)^{1/3} \rho_0^{5/3} \pi \beta c^{-4} \left(1 - \frac{c^2}{b^2}\right) \qquad (2\text{-}2)$$

where $-\beta / r^6$ is the van der Waals potential.

Solving equation (2-1) graphically, he calculates the radius of the bubble to be 12.1 Å.

It is interesting to note that the electrostatic pressure at this radius is less than 10% of P_{kin} and ignoring it would only increase the radius to approximately 12.3. Hence the only effect of polarization is to increase the effective mass of the ion. Kuper has shown that polarization increases the effective mass by 20%. However in any calculation of the structure of the bubble, the polarization can be treated as a correction term.

There are a number of possible errors in Kuper's treatment of the problem, which could significantly affect the radius of the bubble. The first is the estimated correction to the pressure on the bubble from van der Waals forces. As Kuper himself has pointed out, his approximation to the radial distribution function is quite crude and if one uses it to calculate the latent heat per atom, it gives an answer that is 33% too low. If one takes this as an estimate of the uncertainty in the van der Waals pressure, one finds that the radius of the bubble could lie anywhere between the approximate limits 11·3 Å and 13·5 Å, being smaller than 12·1 Å if $|P_{vdW}|$ is overestimated and larger than 12·1 Å if $|P_{vdW}|$ is underestimated.

A second source of error is the assumption that the kinetic energy of the electrons is given by the formula $\pi^2 \hbar^2 / 2\mu b_-^2$. This assumes that the bubble constitutes an infinitely deep well in which the electron is trapped and that there is no penetration by the electrons wave-function into the fluid. This is clearly not the case. The fluid constitutes a well of finite depth of order

$$V_0 = \frac{2\pi \ell \hbar^2}{\mu} \rho_0 \qquad (2\text{-}3)$$

where ℓ is the electron-helium atom scattering length, μ is the electronic mass and ρ_0 is the density of the fluid. The approximation that the well is infinitely deep can only be made if

$$V_0 \gg \frac{\pi^2 \hbar^2}{2\mu b_-^2} \qquad (2\text{-}4)$$

or

$$b_-^2 \gg \frac{\pi}{4\ell\rho_0} \sim (7.1\ \text{Å})^2 \qquad (2\text{-}5)$$

Since this criterion is not completely satisfied there will be a significant overlap of the electrons wave-function and the fluid. Hence there exists the interesting possibility that the electrostatic attractive forces -small at $12.1\ \text{Å}$, but which increase as r^{-4} - may become large more rapidly than the repulsive pressure exerted by the electron and hence reduce the bubble radius to a much smaller value than Kuper found (Gross, 1965). There would then be a finite probability of finding the electron outside the bubble and the electrostatic pressure would no longer be that around a point charge.

Later calculations in this thesis (Chapters 3. and 4.) allow overlap of the wave-functions but find this causes no drastic change in the radius. Hence it appears that the electrostatic attraction is too weak at $12.1\ \text{Å}$ to promote the collapse to a smaller radius mentioned above. Only a detailed comparison of the energies in-

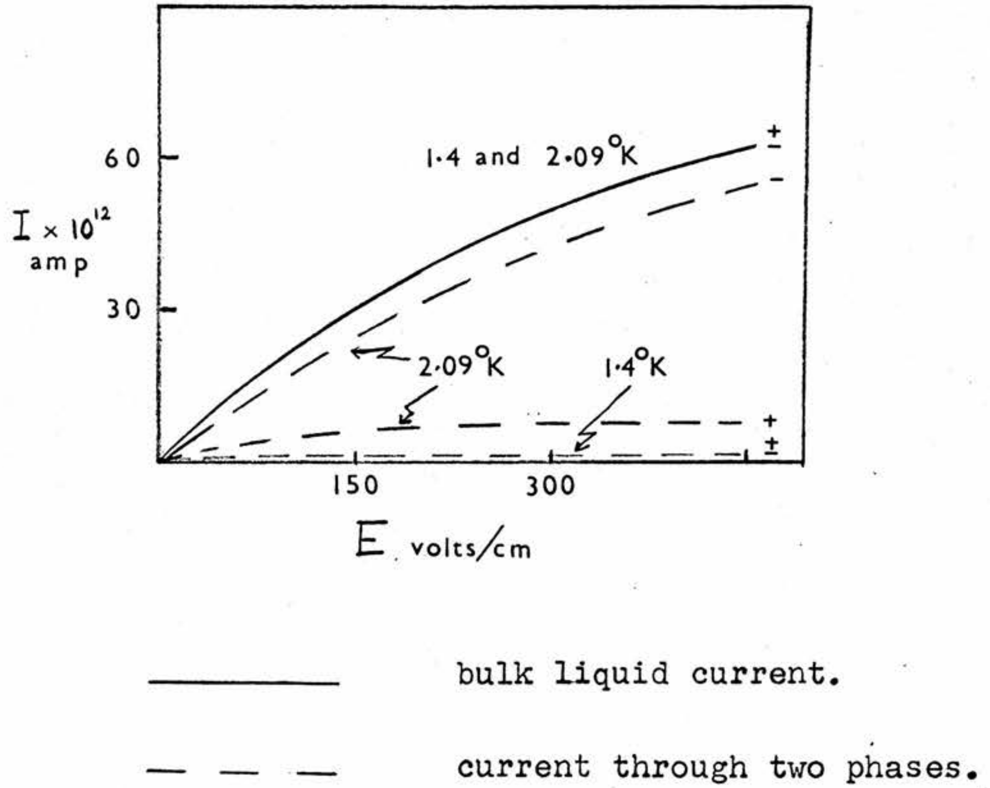


Figure 2.1. (after Careri, 1961).

volved could decide whether the smaller radius bubble is more likely to exist than the larger. Experimentally it may be feasible to decide between the two on the basis of effective masses, scattering cross-sections or excitation energies but the two radii are not sufficiently different to make decisive experiments easy.

2. The Experimental Evidence.

The experimental evidence supporting the bubble model of the negative ion in liquid helium four rests mainly on the behaviour of the ion as it crosses a phase boundary of helium. Careri et alii (1960) performed the earliest experiment of this type, the results of which are shown schematically in Figure 2.1.. The gap between two horizontal plates of a parallel plate condenser were filled or half-filled with liquid helium. On the lower plate was a radioactive layer which ionised the helium in its vicinity and from which ions of either sign could be selected by the appropriate field.

The currents collected at the top plate were measured and plotted as a function of the field across the space. When the space was filled with liquid helium, the currents collected were the same for both positive and negative ions and were approximately independent of temperature. Above the λ -point the currents collected were approximately the same whether the space was filled or only half-filled with liquid helium, but below the λ -point, the positive ion current dropped rapidly with decreasing temperature. The negative ion current, on the other hand, remained high to lower temperatures, though eventually it too disappeared near 1° K .

As Careri pointed out this behaviour of the negative ion can only be satisfactorily explained on the basis of the bubble model. Firstly, since collisions with excitations (rotons) in the liquid are needed to enable either ion to overcome the attractive polarization forces and cross the phase boundary, the decrease in current with temperature is explicable in terms of the drop in roton density with temperature. Secondly, since the negative ion penetrates the surface more easily than the positive, the negative must be a substantially lighter quantity. This, since the positive ion is suspected to be He_2^+, rules out any such models as He_n^- or a negatively charged impurity atom.

Thus it is probable that the negative ion is an electron. The final point made by Careri that the negative ion is trapped at low enough temperatures, argues against the model of a relatively free electron proposed by Davis et alii (1962) for the negative ion in He I. For if the electron moves through the helium with an energy of about 1 eV (see below), it would have this energy available to penetrate the surface on passing out the helium. However if some of this energy has been dissipated in creating a bubble structure, then the electron would be trapped by the surface more readily. This argument makes some physical assumptions about the nature of the energy barrier at the surface but accounts for the experimental result. It would be interesting to measure experimentally the energy required by an electron to penetrate the surface from below for this might shed some light on the above theory.

These considerations have been given some qualitative support by Sommer (1964). Sommer tried to pass electrons into liquid He^4 from the vapour and found that the surface represented a barrier to the passage of electrons of slightly more than 1 eV. If the surface is kept drained of charge and the energy distribution function of the electrons impinging on the surface is known, then a measure of that fraction of the current that penetrates the surface gives an indication of the size of the energy barrier. Sommer calculates the barrier to be about 1·3 eV but estimates that the errors could alter this by 30%.

More recently Woolf and Rayfield (1965) have confirmed Sommers result that the energy required to inject an electron into liquid helium is about one electron volt. By measuring the spectral response of a photocathode both when covered in helium and when in vacuum, they can deduce directly the extra energy needed to inject electrons into liquid helium. They find a value of $1\cdot 02 \pm 0\cdot 08$ eV. This is in very good agreement with the value $1\cdot 09$ eV found by Burdick (1965) theoretically on the basis of a free electron model.

3. The Quasi-Free Electron.

Burdick has calculated the energy of an electron moving in periodic lattice. He considers solutions of the Schrodinger equation for an electron moving through a periodic array of hardcores.

$$(\nabla^2 + k^2)\Psi(\underline{r}) = 4\pi l \sum_{\underline{a}} \delta(\underline{r}-\underline{a}) \frac{\partial}{\partial|\underline{r}-\underline{a}|}\left[|\underline{r}-\underline{a}|\Psi(\underline{r})\right] \qquad (2\text{-}6)$$

Writing $\Psi(\underline{r}) = \sum_{\underline{b}} \phi_{\underline{b}}\, e^{i\underline{b}\cdot\underline{r}}$

where the vectors $\underline{b}$ are 2π times the reciprocal lattice vectors generated by the lattice $\underline{a}$, Burdick shows that

$$\Psi(\underline{r}) = -\frac{16\pi^2 l}{\Delta} \sum_{\underline{b}} \frac{e^{i\underline{b}\cdot\underline{r}}}{b^2 - k^2} \qquad (2\text{-}7)$$

and applies the boundary condition that $\Psi(\underline{r}) = 0$ on the surface of each hard sphere. ($\Psi(\underline{r})$ in

(2-7) is in fact calculated from the equation

$$\left(\nabla^2 + k^2\right)\Psi(\underset{\sim}{r}) = 4\pi \ell \sum_{\underset{\sim}{a}} \delta(\underset{\sim}{r} - \underset{\sim}{a})$$

so that this condition has not been used yet). Borrowing techniques from solid state theory, where similar sums are performed to calculate Madelungs constant, he obtains an algebraic equation for k^2.

Calculations have been performed for various types of lattice; namely simple cubic, body-centered cubic and face-centered cubic. These calculations yield the values $1{\cdot}71$, $1{\cdot}76$ and $1{\cdot}77$ eV respectively for the energy if the scattering-length ℓ is $1{\cdot}46\, a_0$ (where a_0 is the Bohr radius). If $\ell = 1{\cdot}13\, a_0$, the simple cubic lattice gives an energy value of $1{\cdot}09$ eV. All the above energies are calculated with the density chosen to be that of liquid helium.

Thus from both experiment and theory we have a picture of the electron moving as in a lattice immediately after injection. Since the bubble represents a lower energy state, the electron must decay into this state in a time of the order of 10^{-12} sec; this being roughly the time required by the helium atoms to move a distance of the order of the bubble radius (Woolf and Rayfield, 1965). Burdick suggests that in this process the extra energy is dispersed by phonon emission. The analogy with the strongly coupled polaron can be invoked to show that although the electron will take advantage of any density depression in order to aid the transition to the bubble state, there is no energy barrier to be overcome and that the process can proceed spontaneously.

4. The Electron-Helium Atom Scattering Length.

The value $1{\cdot}13\, a_0$ of the scattering length used by Burdick agrees with that found to fit the observed total elastic cross-section of helium atoms for scattering by slow electrons, (O'Malley, 1963). Moreover he, Burdick, calculates a polarization correction to the theoretical scattering length $1{\cdot}46\, a_0$ (Moiseiwitsch, 1953) and shows that it also reduces to $1{\cdot}13\, a_0$. Moiseiwitsch's scattering length calculation includes the effect of exchange but not of polarization. The method used by Burdick is due to O'Malley, Spruch and Rosenberg (1961), who have modified the usual effective range theory for short range potentials to include the 'long range' polarization potential $V(r) = \alpha / r^4$ where α is constant. Here 'long range' means the the potential only falls off at large distances as some power of r^{-1}. The argument is essentially that the radial equation

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{L(L+1)}{r^2} - \frac{2\mu}{\hbar^2} V(r) \right] U(r) = 0 \tag{2-8}$$

does not have solutions which behave asymptotically as linear combinations of solutions of the free particle equation

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{L(L+1)}{r^2} \right) U(r) = 0 \tag{2-9}$$

unless $V(r)$ drops off for large r more rapidly than any power of r^{-1}. In other words for long range potentials it is not valid to drop the $V(r)$ term in determining the asymptotic behaviour of solutions of (2-8).

The knowledge of the asymptotic behaviour of the solutions of (2-8) is essential to the usual method of calculating the phase shifts. The correspondence between the form of the solutions of (2-8) and of (2-9) together with the boundary conditions that $U(r) = 0$ at $r = 0$ defines the phase shift and hence the scattering length and the effective range.

O'Malley, Spruch and Rosenberg observe however that the equation

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{L(L+1)}{r^2} + \frac{\beta^2}{r^4} \right) U(r) = 0 \qquad (2\text{-}10)$$

can be solved exactly, since the equation can be related to Mathieu's equation by the transformation

$$\begin{aligned} r &= \left(\frac{\beta}{k}\right)^{1/2} e^{Y} \\ U(r) &= r^{1/2}\,\phi(Y) \end{aligned} \qquad (2\text{-}11)$$

Hence, if two independent solutions are $V_{pc}(r)$ and $V_{ps}(r)$, then solutions of (2-8) that behave for large r as $V_{ps}(r) + B\,V_{pc}(r)$ may be found if the potential in (2-8) is of the form

$$V(r) = \Delta V(r) + \beta^2/r^4 \qquad (2\text{-}12)$$

where $\Delta V(r)$ is 'short range'. An expression for the phase shift may now be found as the asymptotic forms of $V_{ps}(r)$ and $V_{pc}(r)$ are known and may be compared to the usual form

$$\sin\left[kr - \tfrac{1}{2}L\pi + \eta(L)\right] \tag{2-13}$$

As Burdick (1965) points out if $\Delta V(r)$ is a hard-core potential the application of the above is especially simple for the potential may be replaced by the boundary condition that the radial wave-function vanishes on the hard-core, but satisfies (2-10) everywhere else.

The substitution $y = r^{-1}$ converts (2-10), (in the low energy limit, $k^2 = 0$) into the equation

$$\left(y^2\frac{d^2}{dy^2} + 2y\frac{d}{dy} - L(L+1) + \beta^2 y^2\right)\phi(y) = 0 \tag{2-14}$$

where $\phi(y) = U(r^{-1})$, and this is the equation for the spherical Bessel functions. Hence the solution of (2-10) is

$$j_L(\beta/r) + B_0\, n_L(\beta/r) \tag{2-15}$$

where B_0 is determined by the boundary condition on the surface of the hard sphere. The asymptotic form of this solution $(r \to \infty)$ is

$$\frac{(\beta/r)^{L}}{(2L+1)!!} - B_0 \frac{(\beta/r)^{-(L+1)}}{(2L-1)!!} \qquad (2\text{-}16)$$

Comparison of this with the usual expansion for low energies in terms of the scattering length gives the formula for the modified S -wave scattering length.

$$\begin{aligned} \ell &= -\frac{\beta}{B_0} \\ &= -\beta \frac{n_0(\beta/\lambda)}{j_0(\beta/\lambda)}, = \beta \cot(\beta/\lambda) \end{aligned} \qquad (2\text{-}17)$$

where λ is the hard core radius.

The value of ℓ depends fairly critically on the ratio β/λ , vanishing if $\lambda = \frac{2}{\pi}\beta$ but tending to λ if λ is large.

Now the atomic polarizability of liquid helium $(\cdot 203\ \text{Å}^3)$ gives a value of $\beta = \cdot 619$ Å and if the hard core radius is taken to be the value $\lambda = 0{\cdot}77$ Å which is the value found by Moiseiwitsch (1953) the polarization correction gives

$$\ell = 0.60\,\mathring{A} = 1.13\,a_0 \qquad (2\text{-}18)$$

This value agrees exactly with the experimentally measured value (O'Malley, 1963) as mentioned above.

5. The Positive Ion.

This section will describe briefly the theory of the structure of the positive ion put forward by Atkins (1959, 1963). This theory reveals the strong effect that the polarization forces may have. Around the negative ion the atoms are displaced beyond the effective range of these forces.

Atkins gives good arguments for assuming that the positive ion is He_n^+ where n is a small integer (probably $n = 2$), and hence that the charge is localized to a small region. This being so the electric field around the ion polarizes the atoms. By a straightforward thermodynamic argument, assuming only that the liquid can be treated as a continuum, Atkins shows (see also Durney, 1963) that the molar volume V

of the liquid at pressure p is related to the field E at any point by

$$\int_{p_0}^{p} V\,dp = \int_0^{E} P\,dE = \frac{1}{2} N \alpha_0 E^2 \qquad (2\text{-}19)$$

where p_0 is the pressure at the point where the electric field $E = 0$ and $\underline{P}$ is the polarization vector. Using the Clausius-Mosotti formula, the relation

$$E = \frac{e}{\varepsilon r^2} \qquad (2\text{-}20)$$

where ε is the dielectric constant and r is the distance from the charge, Atkins evaluates the integral approximately (where $p - p_0$ is small) as $V_0 (p - p_0)$. The change in density in this region is,

$$\rho - \rho_0 = \frac{\gamma N \alpha_0 e^2}{2 V_0 u_1^2 \varepsilon_0^2 r^4} \qquad (2\text{-}21)$$

where γ is the ratio of the specific heats; N is Avogadro's number; α_0 is the molecular polarizability; and u_1 is the velocity of first sound.

The pressure and density both increase as r^{-4} as r decreases and at 6.3 Å from the ion the pressure reaches the melting pressure. However as both Atkins and Kuper (1963) remark the continuum approximation breaks down at these distances and there is in fact no reason to believe that a solid-like structure is formed. It is certain that the density is increased over a large distance around the ion and this causes the ion to have a large effective mass. Atkins estimates that about forty helium atoms move with the ion which, if one includes the hydrodynamic mass (Kuper, 1961) leads to a total effective mass of approximately seventy-five helium atom masses. This estimate is based on the assumption that only the part inside 6.3 Å contributes to the hydrodynamic mass, i.e. the quasi-solid part. Gross (1962) has made a more detailed appraisal of the flow pattern around the ion, concluding that it is not simply dipolar but that far in front of the ion atoms move in towards it because of the polarization forces. Gross' treatment leads to very high effective masses $\sim 300\ M_{He^4}$ but as he remarks his approximation to the boson-boson interaction is not realistic enough to warrant drawing more than order of magnitude values from the theory.

Atkins' theory reveals that the polarization forces play a very important part in determining the effective mass of the ion. The detailed structure close to the ion is not clear but this is not critical to the argument. He also originally proposed a similar model for the negative ion on the grounds that the electron might behave as though it were in the bottom of the conduction band of an insulator, and that increasing the density of the helium would lower the energy of the bottom of the band. This idea has yet to be worked out in detail but it seems likely that any energy gained in this fashion would be offset by the higher kinetic energy of the electron. This energy increase is due to the reduction in the space available to the electron between the helium atoms. Presumably Atkins included this change in the kinetic energy when he estimated that the band energy would lowered. He gives no details. However it would be surprising if the total energy was finally lower than the energy of the bubble structure, which involves a similar displacement of the atoms but with a very pronounced reduction in the energy of the electron.

CHAPTER 3.

SOLUTIONS OF THE EQUATION OF MOTION.

In this chapter we shall set up a Hamiltonian that approximates to that of an electron in liquid helium. In this chapter and in most of the rest of the thesis we shall take as a model of the negative ion, a light impurity in a hard-sphere boson system. A hard-sphere system is the best model of liquid helium that is amenable to calculation. Even so, since no mathematical technique has been devised capable of handling it over all ranges of its parameters, it is unphysical in that it requires the system to be both dilute and degenerate. It is not the purpose of this thesis to review its successes and failures but merely to recognise its limitations in particular with respect to the density of the system.

Having stated this limitation we are immediately led into a situation which cannot be glossed over. It will be shown below that the existence of a bubble-like state depends on the strength of the interaction between the bosons and the impurity and hence indirectly on the density. With values of the masses and scattering lengths pertinent to an electron in helium, we find that the minimum density showing a bubble structure is already above the maximum for which our model is valid. This is not as serious as it sounds, for the magnitude of the coupling constant may be taken to be model-independent. In other words, if we use the actual value of the coupling constant of an electron in liquid helium our model shows a bubble structure despite the low density. Hence we feel reasonably justified in extrapolating results found with the model to the real physical problem.

1. Elementary Considerations.

In order to permit mathematically the formation of a bubble-like state in the boson system, we require a formulation of the problem in which the bosons may be described by a spatially inhomogeneous state. Clearly if the bubble is formed and is at rest with respect to the surrounding boson fluid then we may expect the state of the bosons to have spherical symmetry about the bubble centre. Moreover we expect the system to return to its undisturbed state at not very large distances from the bubble. Indeed on the basis of this type of argument we can make a very crude variational estimate of the radius of the bubble.

Assume that the electron is effectively trapped in an infinitely deep spherical well of radius r. Then its energy is just

$$E_e = \frac{\hbar^2 \pi^2}{2\mu r^2} \tag{3-1}$$

Similarly if the only effect on the boson system is to decrease the volume available to it by an amount $V = 4\pi r^3/3$, then the energy of the system is

$$E_b = \frac{4\pi a N^2 \hbar^2}{2M(\Omega - V)}\left[1 + \frac{128}{15\pi^{1/2}}\left(\frac{a^3 N}{\Omega - V}\right)^{1/2}\right] \tag{3-2}$$

where we have used the ground state energy of bosons interacting via a hard short-range repulsive potential derived by many different authors and methods. Since V is small compared to Ω, the volume of the system, equation (3-2) can be written

$$E_b = \frac{4\pi a N^2 \hbar^2}{2M\Omega}\left\{\left[1+\frac{128}{15\pi^{1/2}}\left(\frac{a^3 N}{\Omega}\right)^{1/2}\right] + \frac{V}{\Omega}\left[1+\frac{64}{15\pi^{1/2}}\left(\frac{a^3N}{\Omega}\right)^{1/2}\right] + O\left(\frac{V^2}{\Omega^2}\right)\right\}$$

(3-3)

and the radius of the bubble may be found by minimising $E_e + E_b$ with respect to r. We find

$$r^5 = \frac{M}{8\mu a \rho^2}\left[1 + \frac{64}{15\pi^{1/2}}\left(a^3\rho\right)^{1/2}\right]^{-1}$$

(3-4)

where $\rho = N/\Omega$ is the number density of the bosons. Though the energy (3-2) cannot be applied to liquid helium, it is of interest to calculate r on inserting values of a and ρ that are approximately those of liquid helium. Taking a, the boson diameter, to be $2{\cdot}7\ \mathring{A}$ and ρ to be $(3{\cdot}6\ \mathring{A})^{-3}$ we find the radius of the bubble

$$r \approx 12 \cdot 4 \ \text{Å} \tag{3-5}$$

It is not surprising that this estimate is fairly close to the phenomenological value found by Kuper of $12 \cdot 1$ Å . For the above calculation is merely a refinement of the following physical argument. London (1954) pointed out that the properties of liquid helium at low temperature are essentially due to the zero-point energy of the atoms and the relative feebleness of the attractive forces between them. Indeed he states, that if one treats liquid helium as a system of hard spheres, the energy per atom lies somewhere between Lenz's (1929) value for a low density system

$$E_{ld} = \frac{2\pi \hbar^2 a}{M c^3} \tag{3-6}$$

and a high density limit

$$E_{hd} = \frac{\pi^2 \hbar^2}{2M(R-d)^2} \tag{3-7}$$

where c is the mean interparticle distance, $\rho^{-1/3}$, and $R = 2^{1/6} c$ is the distance between centre of nearest neighbours in a close-packed structure.

Since liquid helium is a fairly dense medium, we will take (3-7) as the energy per atom. Then an approximate value for the radius of the bubble can be obtained by equating the pressure $(\partial E/\partial v)$ exerted outwards by the trapped electron to the pressure $E\rho$ of the bosons inwards on the bubble volume,

$$\frac{\pi \hbar^2}{4 r^5 \mu} = \frac{\pi^2 \hbar^2}{2M(R-d)^2 c^2} \qquad (3\text{-}8)$$

In liquid helium, $R - d \approx \frac{1}{3} c$, so we arrive at the approximate expression for r

$$\left(\frac{r}{c}\right)^5 \simeq \frac{1}{18\pi}\left(\frac{M}{\mu}\right) \qquad (3\text{-}9)$$

or

$$r \simeq \frac{1}{2.2}\left(\frac{M}{\mu}\right)^{1/5} c \qquad (3\text{-}10)$$

Equation (3-10) gives a value of r of

approximately $10\,\mathring{A}$. Now it is clear that what we have done to obtain (3-10) is an approximation to Kuper's method and that the method used to obtain (3-4) is equivalent to it, except insofar as we have used different expressions for the energy per atom.

Expressions (3-4) and (3-10) are however transparent in a manner that Kuper's expression is not. Both show how the radius of the bubble is proportional to the fifth power of the ratio of helium atom mass to the electron mass. The other factors in each expression merely define a significant unit of distance in the boson system, effectively the interparticle distance. This has been deliberately brought out in (3-10) by the substitution $(R-d) \simeq 1/3\, c$.

To develop the elementary treatments given above we need to consider the Hamiltonian of the system.

2. The Hamiltonian.

The Hamiltonian of the electron and the interacting boson system can be written down immediately in configuration space.

$$H = H_b + H_e + H_{be} \tag{3-11}$$

where

$$H_b = -\frac{\hbar^2}{2M}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i>j}\sum V(|\underline{x}_i - \underline{x}_j|)$$

$$H_e = -\frac{\hbar^2}{2\mu}\nabla_e^2$$

$$H_{be} = \sum_{i=1}^{N} W(|\underline{y} - \underline{x}_i|)$$

where the coordinate vector $\underline{y}$ refers to the position of the electron and $\underline{x}_i$ to the i^{th} boson. In writing down this Hamiltonian it has been assumed that only two-body interactions need be considered and that these only depend on the modulus of the relative distance between the interacting bodies. We have also assumed that there are no electron-electron interactions, i.e. the density of the electrons is low enough to merit treating them as single particles.

In order to be able to treat the boson system we have to know its lowest single-particle state. This state will be occupied by the majority of the bosons. The presence of the electron makes it impossible to assume that this state can be described by a wave-function, $\Psi(\underline{r}) =$ const., as is usually done when discussing boson systems. In order to find the ground state we will make a Hartree approximation and assume that the wave-function on which the Hamiltonian (3-11) acts can be written

$$\Psi\left(\underline{y}, \underline{x}_1, \underline{x}_2, \cdots x_N\right) = \phi(\underline{y})\, u(\underline{x}_1)\, u(\underline{x}_2) \cdots u(\underline{x}_N) \tag{3-12}$$

where $\phi(\underline{y})$ and $u(\underline{x})$ are normalized to unity. Using the variational method and evaluating

$$\iint \cdots \int \bar{\Psi} H \Psi \, d^3y\, d^3x_1 \cdots d^3x_N \tag{3-13}$$

where all integrals are over the volume of the total system, we obtain N equations of the form

$$\left[-\frac{\hbar^2}{2M}\nabla_k^2 + \sum_{j \neq k} \int \bar{u}(\underline{x}_j)\, V_{jk}\, u(\underline{x}_j)\, d^3x_j + \int \bar{\phi}(\underline{y})\, W_k\, \phi(\underline{y})\, d^3y\right] u(\underline{x}_k) = \varepsilon_k\, u(\underline{x}_k) \tag{3-14}$$

and one of the form

$$\left[-\frac{\hbar^2}{2\mu}\nabla_e^2 + \sum_j \int \bar{u}(\underline{x}_j)\, W_j\, u(\underline{x}_j)\right]\phi(\underline{y}) = \varepsilon_e \phi(\underline{y}) \tag{3-15}$$

where $V_{jk} = V(|\underline{x}_j - \underline{x}_k|)$ and $W_k = W(|\underline{y} - \underline{x}_k|)$.

These equations can be written, dropping suffixes and substituting $U(\underline{x})$ for $\sqrt{N}\,u(\underline{x})$, as

$$\begin{aligned}\Big[-\frac{\hbar^2}{2M}\nabla^2 + \frac{N-1}{N}\int \bar{U}(\underline{x}')\, V(|\underline{x}-\underline{x}'|)\, U(\underline{x}')\, d^3x' \\ + \int \bar{\phi}(\underline{y})\, W(|\underline{y}-\underline{x}|)\, \phi(\underline{y})\, d^3y\Big] U(\underline{x}) = \varepsilon_j U(\underline{x})\end{aligned} \tag{3-16}$$

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + \int \bar{U}(\underline{x})\, W(|\underline{y}-\underline{x}|)\, U(\underline{x})\, d^3x\right]\phi(\underline{y}) = \varepsilon_e \phi(\underline{y}) \tag{3-17}$$

Equations (3-16) and (3-17) are essentially the same as obtained by Gross (1958) using a semi-classical approach. This is not surprising as the semi-classical approach to the ground-state is completely equivalent to the Hartree one. The Hartree method we have used here makes clear the ideas behind the calculation. We assume that each atom moves in a potential due to all the other atoms and to the electron and that all atoms are in identical states. The electron is assumed to move in a potential due to the presence of the bosons. These potentials are self-consistent in that they depend on the wave-functions $\mathcal{U}(\underline{x})$ and $\phi(\underline{y})$ themselves.

To study equations (3-16) and (3-17) we need to make some assumptions about the nature of the potentials $V(|\underline{x}-\underline{x}'|)$ and $W(|\underline{y}-\underline{x}'|)$. In liquid He II, we would expect them both to consist of a strong short-range repulsion accompanied in the boson-boson case by a van der Waals attractive force and in the electron-boson case by a long range attractive polarization force. In the following exposition we shall assume the repulsive forces to be dominant. The neglect of the polarization forces may be justified by referring to Chapter 2., where their effects were shown to be small. The inclusion of an attractive term of the right magnitude in the computer calculation described below, only altered the solutions within the error range. In neglecting the attractive component of the boson-boson potential, we are departing from reality. Kuper has shown that this can reduce the effective pressure exerted by the atoms on the bubble by more than 50%. To a certain extent we can incorporate the attraction in our definition of the atom-atom scattering length but this is not completely satisfactory. The concept of a uniform negative potential applied externally to the system fails when we have non-uniform systems, for we do not know how to calculate the change in potential at the boundary. That we obtain a radius in good agreement with Kuper's calculation implies that the result is not strongly dependent on the model. The problem, however, really requires an adequate treatment of the effect of the attractive part of the potential.

3. The Model Equations.

As mentioned above the model that will be considered is that of a light particle in an imperfect Bose gas. All interactions will be taken to be purely repulsive and of short-range. The force between the impurity and a boson particle will be assumed to be large compared with the boson-boson interaction. These potentials will be described by the pseudo-potential

$$V\left(|\underline{x}-\underline{x}'|\right) = \frac{8\pi a \hbar^2}{2M}\,\delta\left(|\underline{x}-\underline{x}'|\right) \tag{3-18}$$

and

$$W\left(|\underline{x}-\underline{y}|\right) = \frac{8\pi l \hbar^2}{4\mu}\,\delta\left(|\underline{x}-\underline{y}|\right) \tag{3-19}$$

Here a is the boson-boson scattering length (the hard-core diameter) and l is the impurity-boson scattering length. Since the impurity mass, μ, is assumed to be much less than the boson mass M, ($\mu \ll M$), in (3-19) the reduced mass, $(\mu^{-1} + M^{-1})$, has been replaced by the impurity mass μ.

The use of the potential (3-18) to describe the boson-boson interaction restricts the calculation to low-density systems, for this potential only simulates the hard-core correctly to first-order in the parameter $(a^3\rho)^{1/2}$ in perturbation theoretical calculations of the ground state energy. Within the Hartree approximation made earlier, this first order term is all that could be expected, since no particles are permitted to be in 'excited' states. It is for corrections to this first order energy of the system due to the presence of the impurity that we are looking. The use of the potential (3-18) is consistent with the Hartree approximation for (3-18) is essentially an 'optical approximation'. That is, the rest of the boson system is replaced by a medium having an index of refraction (see Huang, 1963), and the wave-functions required are those of particles moving in this medium.

Inserting the potentials (3-18) and (3-19) in equations (3-16) and (3-17) and dropping a factor of order N^{-1}, they become

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + \frac{8\pi a\hbar^2}{2M}|U(\underset{\sim}{x})|^2 + \frac{8\pi\ell\hbar^2}{4\mu}|\phi(\underset{\sim}{x})|^2 - \varepsilon_b\right]U(\underset{\sim}{x}) = 0 \tag{3-20}$$

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + \frac{8\pi\ell\hbar^2}{4\mu}|U(\underset{\sim}{x})|^2 - \varepsilon_e\right]\phi(\underset{\sim}{x}) = 0$$

(3-21)

Let us look for spherically symmetric solutions of the form

$$\phi(\underline{x}) = R_{1,\ell}(r)\, Y_{1,\ell m}(\theta, \phi)$$

$$U(\underline{x}) = R_{2,\ell}(r)\, Y_{2,\ell m}(\theta, \phi) \tag{3-22}$$

and put $\ell = 0$, so that only the radial dependence of the wave-function is considered. Then writing $\varepsilon_b = \frac{\hbar^2 k_2^2}{2M}$ and $\varepsilon_e = \frac{\hbar^2 k_1^2}{2\mu}$

the equations (3-2o) and (3-21) become,

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR_1}{dr}\right) + \left(k_1^2 - 4\pi\ell\, R_2^2(r)\right)R_1(r) = 0 \tag{3-23}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR_2}{dr}\right) + \left(k_2^2 - 8\pi a R_2^2(r) - 4\pi\ell\left(\frac{M}{\mu}\right)R_1^2(r)\right)R_2(r) = 0 \tag{3-24}$$

with the normalization conditions

$$4\pi \int_0^{\mathcal{R}} R_1^2\, r^2\, dr = 1 \tag{3-25}$$

$$4\pi \int_0^{\mathcal{R}} R_2^2\, r^2\, dr = N \tag{3-26}$$

In equations (3-23) to (3-26) we have assumed that $R_1(r)$ and $R_2(r)$ are real (we are looking for stationary solutions) and we will impose the boundary condition that both wave-functions vanish on the wall of the container, $r = \mathcal{R}$. Of course, since these are radial wave-functions, we only consider solutions that are finite at the origin.

To show that equations (3-23) to (3-26) have solutions that describe a bubble-like structure, let us first consider (3-24) with $R_1 = 0$ i.e. when no electron is present.

$$\frac{d^2 R_2}{dr^2} + \frac{2}{r}\frac{dR_2}{dr} + \left(k_2^2 - 8\pi a R_2^2\right) R_2 = 0 \tag{3-27}$$

This equation should have a nearly uniform solution, with $R_2 = \rho_0^{1/2}$ everywhere except at the wall. If we let the radius of the container become infinite, $\mathcal{R} \to \infty$, then $R_2 = \rho_0^{1/2}$ everywhere satisfies the normalization condition. Equation (3-27) has a solution of this form if $k_2^2 = 8\pi a \rho_0$. The energy of the boson system in this uniform state is $\frac{N}{2} k_2^2$, in units of $\hbar^2/2m$. The factor half arises since we have counted all boson-boson interactions twice in finding Nk_2^2 by the Hartree method.

Equation (3-27) is a very interesting non-linear equation that it would be useful to be able to solve with other boundary conditions than those required for the uniform solution. It is an equation of the type

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + f(R) = 0 \qquad (3\text{-}28)$$

known as Emden type (see Davis, 1960) after the astrophysicist R. Emden who first studied equations of this nature in 1907. We discuss this equation more fully in Appendix A . Here, all we need to know is that there exist solutions of (3-27) that behave like the uniform solution at large distances from the origin but which vanish at some finite distance from the origin.

Now we can give a qualitative description of the bubble-like solutions of (3-23) and (3-24). Let us relax the boundary condition at $r = \mathcal{R}$ and assume simply that $R_2(r) \rightarrow \rho_0^{1/2}$ and $R_1(r) \rightarrow 0$

as $r \to \infty$. Also assume that $R_2(0) \simeq 0$ and $R_1(0)$ is so large that

$$4\pi\ell\left(\frac{M}{\mu}\right) R_1^2(0) \gg k_2^2 \tag{3-29}$$

We can take $\frac{dR_1}{dr} = 0$ and $\frac{dR_2}{dr} = 0$ at the origin. Then $R_1(r)$ behaves approximately as $\sin k_1 r / r$ and $R_2(r)$ remains small but steadily increasing until such a radius that

$$4\pi\ell\left(\frac{M}{\mu}\right) R_1^2 \approx k_2^2 \tag{3-30}$$

(the classical turning-point). At this radius $R_2(r)$ increases rapidly with r, but the term $8\pi a R_2^2$ has the effect of turning the wave-function to the asymptotic value $\rho_0^{1/2}$. $R_1(r)$ on the other hand behaves like the wave-function of a particle seeing a finite potential step and decays exponentially to zero. Note we must have $k_1^2 < 4\pi\ell\rho$ for this behaviour.

Solutions of this form, if they exist, describe the ground state of the system since we have assumed that the wave-functions have no nodes.

Equations (3-23) and (3-24) have been studied on an analogue computer and solutions of the type described above have been shown to exist. The programming and details of the techniques used are discussed in the next section. The results are displayed in Figure 3.2..

4. Analogue Computer Calculations.

An analogue computer provides a rapid and convenient way of analysing non-linear differential equations such as (3-25) and (3-26). The independent variable on the machine is time, t, and the dependent variables, in our case $R_1(r)$ and $R_2(r)$, are calculated as functions of time progressively from some initial value. The technique is most useful when the solutions are stable. Stability can be rigorously defined for an analogue computer by Liapunov's definition, i.e. a solution $\underline{x}(t)$ of a differential equation

$$\frac{d\underline{x}}{dt} = f(\underline{x}, t) \tag{3-31}$$

is stable if for each $\epsilon > 0$, there exists a $\delta > 0$ such that any solution $\underline{y}(t)$ of (3-31) satisfying $\|\underline{x} - \underline{y}\| \leq \delta$ for $t = 0$ also satisfies $\| \underline{x} - \underline{y} \| \leq \epsilon$ for all $t \geqslant 0$. Here $\| \underline{x} \| = \sum_{i=1}^{n} | x_i |$, where $\underline{x}$ is an n-dimensional vector.

Now the set of equations (3-23) to (3-26) have boundary conditions at both ends of the interval over which we wish to calculate R_1 and R_2. For we are given $dR_1/dr = dR_2/dr = 0$ at $r = 0$ and also $R_1 = R_2 = 0$ at $r = \mathcal{R}$. Therefore we have to calculate the solutions starting from some trial values of $R_1(0)$ and $R_2(0)$ and vary these initial values until we find the solutions that satisfy the boundary conditions at $\mathcal{R}$. Moreover from these solutions, we have to select those satisfying the integral conditions (3-25) and (3-26) by varying k_1 and k_2 until the correct solutions are found.

The equations are simplified somewhat if we let N and $\mathcal{R} \to \infty$. At distances far from the origin ($r \gg b$ the bubble radius) we expect $R_1(r)$ to be negligible and $R_2(r)$ to have the value $\rho_0^{1/2}$. Hence we can set $k_2^2 = 8\pi a \rho_0$ and neglect the normalization condition (3-26) since corrections to k_2^2 due to the finite size of the bubble will be of order N^{-1}. Thus we can replace (3-26) and $R_2(\mathcal{R}) = 0$ by the single condition that $R_2(r) \to \rho_0^{1/2}$ as $r \to \infty$.

Now the solution $R_2(r) = \rho_0^{1/2}$ to (3-24) is unstable as is shown in the Appendix. Also we are looking for solutions of (3-23) that behave like $r^{-1} e^{-Kr}$ for large r and these are also unstable. This is easily demonstrated if we assume that $R_2(r) = \rho_0^{1/2}$ for all $r > f > 0$ say. Then (3-23) becomes

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR_1}{dr}\right) - K^2 R_1 = 0 \qquad (3\text{-}32)$$

where

$$K^2 = \left(4\pi \ell \rho_0 - k_i^2\right) \qquad (3\text{-}33)$$

Letting $R_1 = \frac{1}{r}\chi$, we have

$$\frac{d^2}{dr^2}\chi_1 = K^2 \chi_1 \qquad (3\text{-}34)$$

which has solutions $\chi_1 = Ae^{Kr} + Be^{-Kr}$.

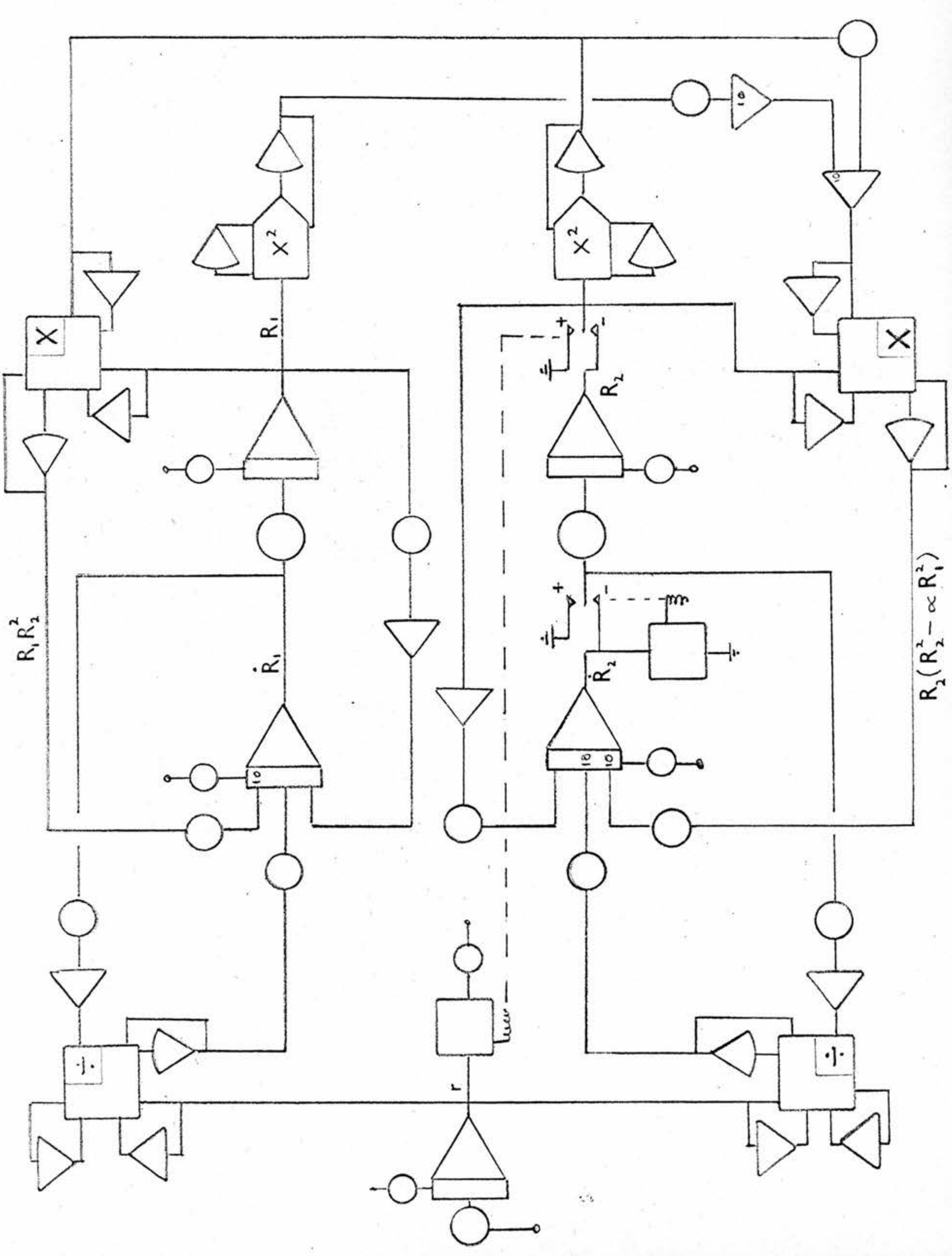
Let $\underline{x} = Be^{-Kr}$, and $\underline{y} = \delta e^{K(r-f)} + Be^{-Kr}$; $\delta > 0$, then $\|\underline{x} - \underline{y}\| = \delta$ at $r = f$, but $\|\underline{x} - \underline{y}\| = \delta e^{K(r-f)}$ for $r > f$ so given $\epsilon > 0$ we can always find a value of r such that

$\| \underline{x} - \underline{y} \| > \epsilon$ irrespective of the value of δ. Thus the solutions are unstable.

The significance of this instability on the analogue computer, is that it is impossible to set up equation (3-32) and to choose the initial conditions on R_1 and dR_1/dr (or equivalently on χ, and $d\chi_1/dr$) such that the computer plots the solution $R_1 = Be^{-Kr}/r$. Any small error in the initial conditions, such as are inherent in an analogue computer, results in an exponentially accumulating error in the solution.

This error can be largely avoided in the region of interest by careful setting of the parameters so that δ is close to zero. But this in itself would not ensure sufficient accuracy. To obtain this we break the interval over which we calculate into two parts. For r larger than some value, q, we can calculate with increasing r and for r less than q, we can calculate backwards to the origin with decreasing r. Although we have now two extra parameters to vary, the fact that the controlled values of the functions and their derivatives are closer to the

Figure 3.1.


X^2
X^2
X
X
R_1
R_2
$\dot{R}_1$
$\dot{R}_2$
$R_1 R_2^2$
$R_2(R_2^2 - \alpha R_1^2)$
r
10
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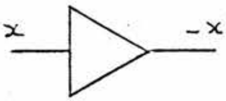
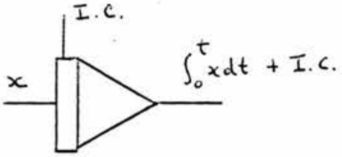
region of divergence means that we can trace the critical solution with much greater accuracy.

This procedure was adopted and the critical solution was held in the unstable region by using a cut-off where this was necessary. The function that diverged most rapidly was the function $R_2(r)$ and this, for $r > g$, was held to its maximum value $R_2(max)$ as soon as its derivative vanished. The parameters were chosen to ensure $R_2(max) \simeq \rho_0^{1/2}$. For $r < g$, r itself was used to switch the comparator and $R_2(r)$ was held to zero for all r less than the value where both R_2 and dR_2/dr were small simultaneously.

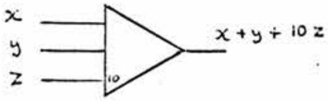
The circuit diagram is shown in Figure 3.1.. The symbols used are defined as follows :



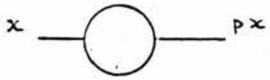
denotes an amplifier used as an inverter.



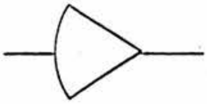
denotes an amplifier used as an integrator.



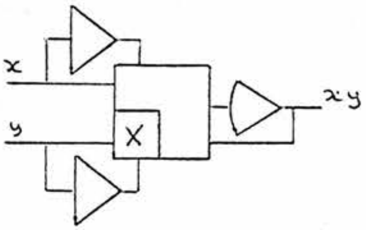
denotes an amplifier used as a summer. (The gain is indicated if it is not unity).



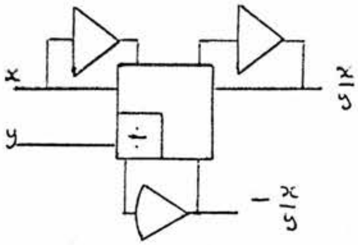
denotes a potentiometer. (Note p is necessarily < 1).



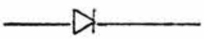
denotes an amplifier in high-gain mode.



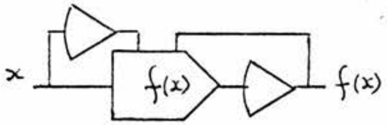
denotes a quarter-square multiplier used to produce a product.



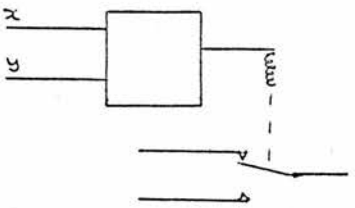
denotes a quarter- square multiplier used to produce a quotient.



denotes a solid state diode



denotes a diode function generator.



denotes a comparator. (The relay switches when $x+y$ passes through zero).

Figure 3.1. does not show the switching mechanism incorporated to enable rapid changing from computing for $r \geqslant g$, the breakpoint, to computing for $r \leqslant g$. Nor is the simple circuit that evaluates the integral, $I(r) \equiv \int_0^r R_1^2 t^2 \, dt$ shown in the diagram. The variables marked in the diagram are unscaled and only indicate the proportional variation of the voltage at that point.

·5. Scaling and Procedure.

The equations (3-23) and (3-24) are not conveniently scaled for setting up on the computer. If we take as a unit of length, $r_0 \equiv (8\pi a \rho_c)^{-1/2}$, the equations become

$$R_1'' + \frac{2}{r} R_1' + \left(k_1^2 - \frac{\ell}{2a} R_2^2\right) R_1 = 0 \qquad (3\text{-}35)$$

$$R_2'' + \frac{2}{r} R_2' + \left(1 - R_2^2 - \ell\left(\frac{M}{\mu}\right) R_1^2\right) R_2 = 0$$

(3-36)

where we have also written R_2 for $\rho_0^{1/2} R_2$ and R_1 for $(4\pi r_0^3)^{1/2} R_1$ so that all the terms are dimensionless. The normalization condition is, in these units :

$$\int_0^\infty r^2 R_1^2 \, dr = 1$$

(3-37)

On an analogue computer all explicit variables are represented by a voltage that must not exceed a certain maximum. On the PACE TR 48 computer this maximum is 10 volts, so we could choose variables that have a maximum modulus of 10.

It is more convenient however to call 10 volts, one machine unit, and to scale the variables to a maximum of unity. Rough approximations were taken at first for the ranges of the variables and these were refined as the nature of the solutions became apparent. The final scaled variables selected were

a) $(10 R_1)$ b) $(2 \times 10^2 \dot{R}_1)$ c) $(2\dot{R}_2)$

d) (R_2) e) $(.04 r)$

Each of these quantities lay in the range $-1 \leqslant x \leqslant 1$ over all the region of computation.

The breakpoint g was chosen at $(\cdot 04\, r) = \cdot 55$ and the integral was evaluated at the maximum range of r, $r = 25$. At this distance R_1 had dropped to a very small value and the integral was virtually constant. Several runs were made with different values of g to ensure that the solution did not depend on the chosen breakpoint.

The procedure adopted to find these values was the following :

1. To obtain approximate solutions, it was possible to switch the computer into its slowest Rep-Op mode in which it continuously cycled from $r = g$ to $r = 25$ or from $r = g$ to $r = 0$ depending on which section had been chosen. In this mode the parameters could be varied manually, watching the functions on a oscilloscope, until the boundary conditions were roughly satisfied. Because of the unstable nature of the solutions, only approximations to them could be found in Rep-Op mode.

2. The computer was switched to Operate and $R_1(\rho)$, k_1 and $R_1'(\rho)$ were varied to make $R_1(r)$ show the correct behaviour as $r \to 0$ and as $r \to \infty$. $R_2(\rho)$ and $R_2'(\rho)$ were then varied to ensure that $R_2(r)$ satisfied its boundary conditions and $R_1(\rho)$ and $R_1'(\rho)$ readjusted if necessary. The solutions were then plotted on an $X-Y$ plotter and the value of the integral read off.
3. k_1^2 was varied to increase or decrease the integral and the procedure repeated. Although tedious, with a little practice, it became possible to find solutions satisfying the boundary conditions fairly rapidly.

6. Errors and Limitations.

The main source of error in the analogue solutions of equations (3-35) and (3-36) lies in the very large constant $\ell\left(\frac{M}{\mu}\right)$, and in the nonlinearity of the equations. On an analogue computer, generation of products or squares of variables is effected by diode-function generators. These function generators are set to produce an output voltage that is the square of the input voltage by means of diodes biased to conduct at preset potentials. The PACE TR 48 quarter-square multipliers have seven diodes to cover the range 0-10 volts, which implies that a parabola is approximated by seven straight line segments. Thus, if the output voltages are low the errors are high and the makers only claim an accuracy of 0.25% of full scale voltage. Hence below 0·5 volts output the accuracy is less than 5% and the multipliers should not be used below this voltage. (Multiplication in a quarter-square multiplier is performed by using the identity

$$xy = \frac{1}{4}\left[(x+y)^2-(x-y)^2\right] \qquad (3\text{-}39)$$

Hence the name).

Unfortunately the critical product in the equations, the term $\ell\left(\frac{M}{\mu}\right)R_1^2R_2$ is such that R_2 is small when R_1^2 is large and R_1^2 is small when R_2 is large. This meant that the output of the multiplier was always small (the variables are scaled so that they never exceed one machine unit) and hence optimum scaling was necessary. This was effected by the device of overloading the multiplier in the 'uninteresting' region where $R_2 = 0$. The variable R_1^2 (scaled) was only greater than $0{\cdot}1$ machine units when $R_2 = 0$. Thus it was possible to multiply it by a factor ten to ensure maximum sensitivity of the multiplier in the region where its output had most effect.

Note since the solutions were computed backwards towards the origin from the breakpoint g, the overloading of the amplifiers had no effect on the results whatsoever. If the solutions had been computed forwards, with r increasing, the amplifiers would have had to come out of an overloaded condition, which takes an appreciable time. Thus the results would have been meaningless.

Despite this improvement, the output of the multiplier would still have been low, since the scaled variables were always less than unity and one or the other was small over the whole interesting range. This was partially avoided by producing in the same multiplier the term R_2^3, as is shown in Figure 3.1.. This meant that at least one of the inputs was close to unity over the full working range of the multiplier and at the same time was physically satisfying as it is just the sum of these two terms, $R_2^3 + \frac{\ell M}{\mu} R_1^2 R_2$ that determines the behaviour of the function R_2.

An inaccuracy that does not affect the nature of the solutions but could cause numerical errors is involved in evaluation of the normalization integral

$$I = \int_0^\infty r^2 R_1^2 \, dr \tag{3-40}$$

Here again we needed to generate $r^2 R_1^2$, in a multiplier the output of which became small as $R_1^2 \to 0$. Once again since we had the breakpoint at $r = g$ we could rescale R_1^2 in the region where r was greater than g to produce more accurate results for that part of the integral in this range. However, the errors involved in evaluating the integral are estimated to be $\pm 2\%$. This error did not give rise to a large error in the wave-functions.A number of runs were made with the calculated value of the integral lying within $1{\cdot}0 \pm 0{\cdot}05$ and the difference in the values of the wave-functions for any given r, was found to be less than 2%. Rather closer limits can be given to the error in the value of k_1^2, as the scaling was such that $20k_1^2$ was actually set on the potentiometer. For k_1^2, the error is estimated as approximately 1%.

It is worth noting that the instability of the wave-functions did not limit the accuracy with which solutions could be found, for the solution that was the critical one between diverging ones was, in fact, quite definite. At $r=0$, the terms $\frac{2}{r}\frac{dR}{dr}$ in the equations caused the slope to change rapidly ($\frac{d^2R}{dr^2}$ became infinite) unless the correct solution was found. This divergence made the correct solution more definite than it would have been had the others not diverged. It was only when R_2 tended to unity or when R_2 tended to zero, where the solutions were so unstable that we were forced to use a cut-off, that errors arose. Close to cut-offs the computed function R_2 is undoubtedly inaccurate and we can only imply that this function approximates to the solution of equation (3-36) in this region. In this next chapter, it is shown that

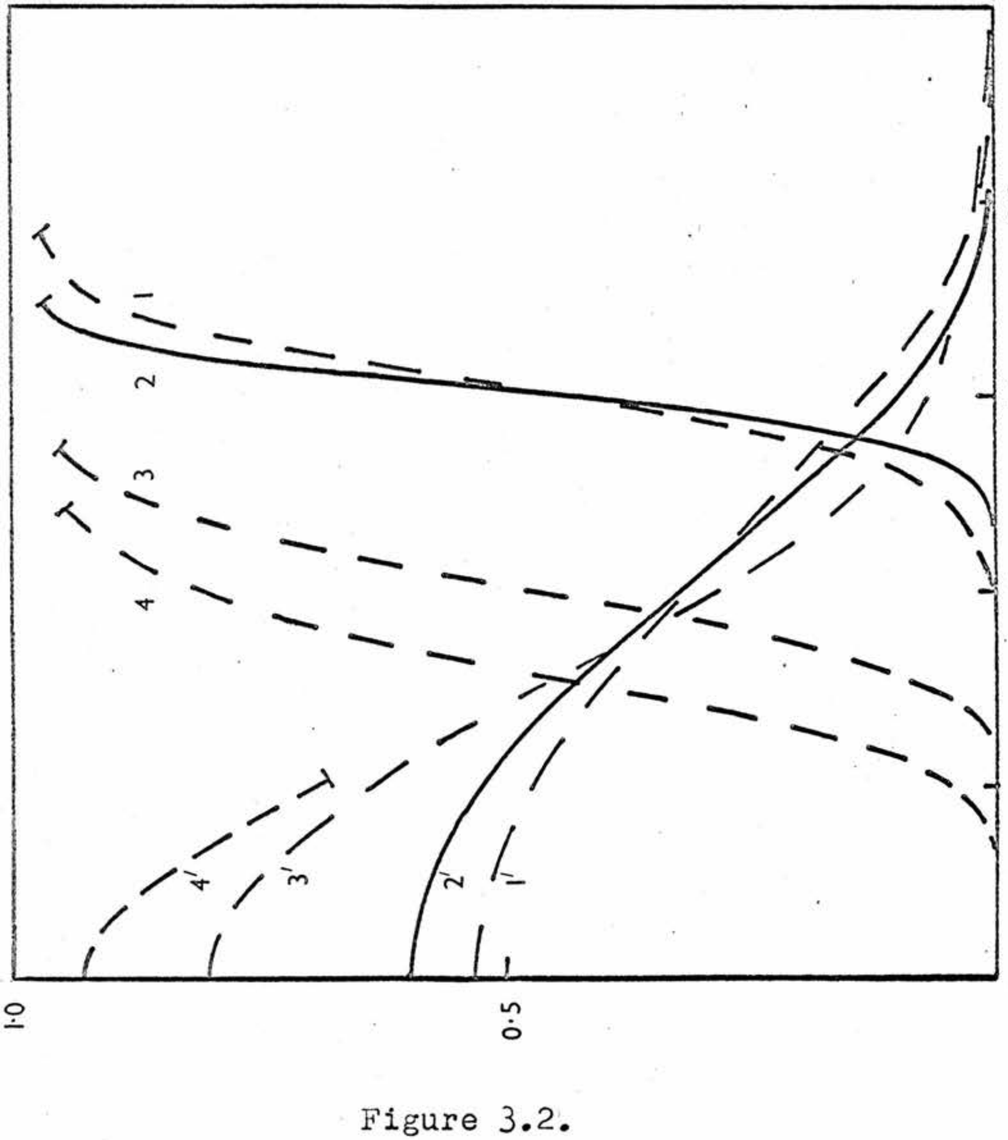


Figure 3.2.

wave-functions of approximately this form do constitute a minimum in the energy of the system and this energy is evaluated.

The solutions have been computed for a number of values of the parameter $\alpha = \frac{\ell M}{\mu}$ and for two values of ℓ for given a and M/μ. It should be remembered that we have taken r_c to be unity and hence decreasing α is equivalent to decreasing the density of the boson system as well as decreasing the mass-ratio. In the next chapter a minimum value for α , giving solutions of the type shown in Figure 3.2. is calculated. The value of k_1^2 , for each value of the parameters is shown in Table 3.1..

In Figure 3.2. the curves labelled 1, 2, 3, 4, are the dimensionless functions R_2 corresponding to the values of α and δ in Table 3.1.. The curves labelled 1', 2', 3', 4', are the complementary solutions R_1 . The x-axis shows distance from the origin in units of r_0 .

The behaviour of the functions for the different values of the parameters is readily understood quantitatively. For small α , which cor-

TABLE 3.1

	α	$\frac{\ell}{a}$	$r_0^2 k_1^2$
1	5.24×10^3	.222	.0275
2	1.18×10^4	.50	.0314
3	1.0×10^3	.222	.0497
4	5.0×10^2	.222	.0651

responds to large impurity particle mass, or low scattering cross-section the bubble radius is small. Increasing ℓ for a given mass-ratio results in a steepening of the wave-functions but no effective change in the radius.

The particular choices of α and ℓ/a were governed partly by the need to equate the model to the only known physical system, that of an electron in He II. If we take $\rho_0 = 2{\cdot}2 \times 10^{22}\ \mathrm{cm}^{-3}$, M/μ as the ratio of a helium atom mass to the electronic mass and a as $2{\cdot}7\ \mathring{A}$, we have for the two values $\ell = \frac{1}{2} a$ and $\ell = {\cdot}222a$, $\alpha = 1{\cdot}18 \times 10^{4}$ and $5{\cdot}24 \times 10^{3}$ respectively. The value $\ell = {\cdot}22a$ is the experimentally determined electron-helium atom scattering length. The lower values of α were chosen with the intention of seeing whether approaching the limit of applicability of the model was detectable as pronounced instability. This was verified.

CHAPTER 4.

THE SELF-ENERGY OF THE ION.

1. A Variational Estimate of the Energy.

To obtain an estimate of the energy of the electron-bubble structure we minimise the energy

$$E = \frac{\int \bar{\Psi} \, H \, \Psi \, d^3x_1 \ldots d^3x_N \, d^3y}{\int \Psi \, \Psi \, d^3x_1 \ldots d^3x_N \, d^3y} \tag{4-1}$$

The Hamiltonian H is given by (3-11) and the potentials by (3-18) and (3-19).

$$H = -\frac{\hbar^2}{2M} \sum_{i=1}^{N} \nabla_i^2 + \frac{8\pi a \hbar^2}{2M} \sum_{i>j} \delta(\underline{x}_i - \underline{x}_j) - \frac{\hbar^2}{2\mu} \nabla_y^2 + \frac{8\pi \ell \hbar^2}{4\mu} \sum_i \delta(\underline{y} - \underline{x}_i) \tag{4-2}$$

The many-particle wave-function $\Psi(\underline{x}_1 \cdots \underline{x}_N, \underline{y})$ may again be taken to be the product wave-function

$$\Psi = \phi(\underline{y}) . N^{-N/2} \, U(x_1) \cdots U(x_N) \tag{4-3}$$

where $\int \phi^* \phi \, d^3_y = 1$ and $\int U^* U \, d^3_x = N$.

The choice of trial wave-functions may be governed by the results of the preceeding section, for the 'best' wave-functions are those plotted in Figure 3.2.. For the boson radial wave-function an expression is needed that behaves approximately like the Fermi-Dirac distribution function substracted from unity

$$U(\underline{r}) = B\left[1 - \left(e^{(r-b)/\tau} + 1\right)^{-1}\right]$$

$$= B\left[1 + e^{-(r-b)/\tau}\right]^{-1} \qquad (4\text{-}4)$$

while for the electron wave-function, we need an expression that behaves as $r^{-1} \sin kr$ near the origin and as e^{-kr} as $r \to \infty$. On the other hand, the choice must be tempered by our ability to perform the integrals and the minimisation, so we choose for $\phi(r)$ the function

$$\phi(\underline{r}) = A(1 + \gamma r)\, e^{-\gamma r} \qquad (4\text{-}5)$$

For $U(\underline{r})$ the choice (4-4) leads to integrals that can only be performed if we make use of the Sommerfeld expansion for this type of integral, i.e.

$$\int_0^\infty \frac{\phi(x)\,dx}{e^{(x-b)/\tau}+1} = \int_0^b \phi(x)\,dx + \frac{\pi^2\tau^2}{6}\phi'(b) + \cdots \tag{4-6}$$

However this is only valid if $\phi(x)$ is slowly varying over a range of width τ about $x = b$ and the function (4-5) is not sufficiently slowly varying. Hence we choose for $U(r)$ a function for which the integrals can be evaluated exactly

$$\begin{aligned} U(r) &= B\left(1 - e^{-(r-b)/\tau}\right); \quad r > b \\ &= 0 \qquad\qquad\qquad\quad ; \quad r \leqslant b \end{aligned} \tag{4-7}$$

Inserting these choices in (4-1) to (4-3) gives

$$\begin{aligned} E = 4\pi\Big[& \frac{\hbar^2}{2M}\int_0^R \left(\frac{\partial U}{\partial r}\right)^2 r^2 dr + \frac{4\pi a\hbar^2}{2M}\int_0^R U^4 r^2 dr \\ & + \frac{\hbar^2}{2\mu}\int_0^R \left(\frac{\partial \phi}{\partial r}\right)^2 r^2 dr + \frac{8\pi\ell\hbar^2}{4\mu}\int_0^R U^2\phi^2 r^2 dr \Big] \end{aligned} \tag{4-8}$$

In all the above integrals the radius of the container $\mathcal{R}$ may be let tend to infinity without complication, except in the second integral where there is a term of the form

$$\frac{16\pi^2 a\hbar^2}{2M}\int_0^{\mathcal{R}} B^4 r^2\,dr = \frac{1}{3}\mathcal{R}^3 B^4 \left(\frac{16\pi^2 a\hbar^2}{2M}\right) \tag{4-9}$$

Now $4\pi B^2 \int_0^{\mathcal{R}} U^2 r^2\,dr = N = \rho_0 \Omega$ from the normalisation condition so

$$B^2 = \rho_0\left[1 - \frac{b^3}{\mathcal{R}^3} - \frac{3\tau^3}{\mathcal{R}^3}\left(\frac{3}{2}\frac{b^2}{\tau^2} + \frac{7}{2}\frac{b}{\tau} + \frac{15}{4}\right)\right] \tag{4-10}$$

Hence if we let $\mathcal{R}\to\infty$, the effect of (4-9) is to contribute to the energy two terms ;

$$\frac{4\pi a\hbar^2}{2M}\rho_0 N + \frac{16\pi^2 a\hbar^2\rho_0^2}{2M}\left[\frac{2}{3}b^3 + 2\tau^3\left(\frac{3}{2}\frac{b^2}{\tau^2} + \frac{7}{2}\frac{b}{\tau} + \frac{15}{4}\right)\right] \tag{4-11}$$

The first being the energy of the undisturbed boson system and the second a contribution to the total energy due the decrease in the volume available to the bosons.

The remaining integrals can easily be evaluated in terms of incomplete gamma functions of integral argument. The normalisation constant of $\phi(\underline{r})$ is

$$A = \left(\frac{\gamma^3}{7\pi}\right)^{1/2} \qquad (4\text{-}12)$$

The expressions simplify if a change of variable is made. Writing $y = b/\gamma$ and $x = \gamma b$ so that x and y are dimensionless and putting, as in Chapter 3.,

$$r_0 = \left(8\pi a \rho_0\right)^{-1/2} = 1$$

the energy (4-8) becomes

$$E - \frac{\hbar^2}{2M}\cdot\frac{N}{2}$$

$$= \frac{\hbar^2}{2M}\cdot\frac{1}{2a}\left[\frac{b}{4y}\left(1+2y+2y^2\right) + \frac{b^3}{2}\left(\frac{1}{3}+\frac{11}{12y}+\frac{89}{72y^2}+\frac{635}{864y^4}\right)\right.$$

$$\left. + \frac{6}{7}\frac{\alpha}{8}\frac{x^2}{b^2} + \frac{\alpha}{56}\int_{2x}^{\infty}(2+t)^2 e^{-t} t^2 dt + \frac{4\alpha}{7}\left\{F(x,\omega) - 2F(x,z)\right\}\right] \qquad (4\text{-}13)$$

where

$$F(x,\omega) = \frac{x^3 e^{-2x}}{\omega^3}\left\{2!\, e_2(\omega) + \frac{2x}{\omega}\, 3!\, e_3(\omega) + \frac{x^2}{\omega^2}\, 4!\, e_4(\omega)\right\}$$

$$e_n(\omega) = 1 + \omega + \frac{\omega^2}{2!} + \cdots + \frac{\omega^n}{n!}$$

$$z = (2x + y) \qquad (4\text{-}14)$$

$$\omega = 2(x+y)$$

and α is the coupling constant defined in the last chapter

$$\alpha = \frac{\ell M}{\mu}$$

and $$\delta = \ell / a \qquad (4\text{-}15)$$

Differentiating E with respect to b , x and y , and equating the results to zero, we obtain

$$A_{(y)} + b^2 B_{(y)} = \frac{12\alpha}{7\delta} \cdot \frac{x^3}{b^3} \qquad (4\text{-}16)$$

$$b\, C_{(y)} + b^3 D_{(y)} = \frac{4\alpha}{7} H(x, y) \qquad (4\text{-}17)$$

$$\frac{12\alpha}{7\delta} \cdot \frac{x^2}{b^2} = \frac{4\alpha}{7} G(x, y) \qquad (4\text{-}18)$$

where $$A_{(y)} = \frac{1}{2}\left(y + 1 + \frac{1}{2y}\right) \qquad (4\text{-}19)$$

$$B_{(y)} = \frac{1}{2}\left(1 + \frac{11}{4y} + \frac{89}{24y^2} + \frac{635}{288y^3}\right) \qquad (4\text{-}20)$$

$$C_{(y)} = \frac{\partial A}{\partial y} = \frac{1}{2}\left(1 - \frac{1}{2y^2}\right) \qquad (4\text{-}21)$$

$$D_{(y)} \equiv \frac{1}{3}\frac{\partial B}{\partial y} = -\frac{1}{2}\left(\frac{11}{12y^2} + \frac{89}{36y^3} + \frac{635}{288y^4}\right) \qquad (4\text{-}22)$$

$$H(x,y) \equiv -\frac{\partial}{\partial y}\left[F(x,\omega) - 2F(x,z)\right]$$

$$= -e^{-2x}x^3\left[2(1+x)^2\left(\frac{1}{z^2}-\frac{1}{\omega^2}\right) + 8(1+x)(1+2x)\left(\frac{1}{z^3}-\frac{1}{\omega^3}\right)\right.$$

$$+ 12(1+6x+6x^2)\left(\frac{1}{z^4}-\frac{1}{\omega^4}\right) + 96x(1+2x)\left(\frac{1}{z^5}-\frac{1}{\omega^5}\right)$$

$$\left. + 240x^2\left(\frac{1}{z^6}-\frac{1}{\omega^6}\right)\right] \qquad (4\text{-}23)$$

and

$$G(x,y)$$

$$\equiv x^3(1+x)^2e^{-2x} - x\frac{\partial}{\partial x}\left[F(x,\omega) - 2F(x,z)\right]$$

$$= x^3(1+x)^2e^{-2x} + x^3e^{-2x}\left[(3+3x-2x^2)(1+x)\left(\frac{2}{z}-\frac{1}{\omega}\right)\right.$$

$$+ (6+18x+4x^2-10x^3)\left(\frac{2}{z^2}-\frac{1}{\omega^2}\right) +$$

$$(6+36x+12x^2-40x^3)\left(\frac{2}{z^3}-\frac{1}{\omega^3}\right) + 12x(3+2x-10x^2)\left(\frac{2}{z^4}-\frac{1}{\omega^4}\right)$$

$$\left. + 24x^2(1-10x)\left(\frac{2}{z^5}-\frac{1}{\omega^5}\right) - 240x^3\left(\frac{2}{z^6}-\frac{1}{\omega^6}\right)\right] \qquad (4\text{-}24)$$

The variable ƀ can readily be eliminated from equations (4-16) to (4-18) giving the equations in x and y :

$$\frac{HA-GC}{GD-HB} = \frac{3}{\delta}\frac{x^2}{G} = \left(\frac{4\alpha}{7}\right)^2\frac{(GD-HB)^2}{\Delta^2} \qquad (4\text{-}25)$$

where $\Delta \equiv AD - BC$. These equations have to be solved numerically. This is more easily done if we rearrange the equations so that the left-hand sides depend largely on y and the right-hand sides on x . This can be usefully done provided $y > x$. The equations actually solved were

$$\frac{(GD - HB)}{x^3 e^{-2x}} = \frac{\delta}{3}\left(\frac{HA - GC}{x^3 e^{-2x}}\right)\frac{G}{x^2} \qquad (4\text{-}26)$$

and

$$\Delta^2 = \frac{16\alpha^2\delta^3}{189}\,\frac{(HA - GC)^2 G^3}{x^6} \qquad (4\text{-}27)$$

The solution was found to be approximately

$$\begin{aligned} x &= 2.84 \\ y &= 4.30 \end{aligned} \qquad (4\text{-}28)$$

which gives for b , γ and τ

$$\begin{aligned} b &= 12.57\ r_0 \\ \gamma^{-1} &= 4.42\ r_0 \\ \tau &= 2.92\ r_0 \end{aligned} \qquad (4\text{-}29)$$

where α and δ have been taken to have the values

$$\begin{aligned} \alpha &= 5\cdot 24 \times 10^{3} \\ \delta &= \cdot 222 \end{aligned} \qquad (4\text{-}30)$$

Figure 4.1. shows the wave-function used above with the calculated values of b , γ and τ and also for comparison the computed solutions for the same values of α and δ . The solid curves are the computed solutions and the dashed curves the variational ones. The solid vertical line is the position of the step found variationally if a step-function is used for $u(r)$. The difference between the two sets of curves shows that the wave-functions (4-5) and (4-7) could probably be greatly improved. The function $(1+\gamma r)\, e^{-\gamma r}$ is too sharply peaked at the origin. The function

$$\phi(r) = A\left(1+\gamma r + \delta r^{2}\right) e^{-\gamma r} \qquad (4\text{-}31)$$

as used by Pekar (1946), would simulate the behaviour near the origin better but the extra parameter would make the minimisation procedure more difficult and tedious. Moreover the improvement in the value of the energy obtained would probably be small. Pekar (1951) remarks that in the polaron theory, (4-31) improves the energy over (4-7) by only 2%, and this can be taken as an indication of the order of magnitude of the difference one might expect.

Better wave-functions for the boson ground state are not hard to guess, but difficult to use in practice. The function (4-4) is one such. In order to obtain an estimate of how important the choice of wave-function is, we can minimise the energy using a step-function for the boson system and (4-7) for the impurity. This is equivalent to putting $y = \infty$, in the above and ignoring the infinite surface energy term. The results for the two sets of wave-functions used are shown in Table 4.1.. The energy of the impurity-boson system is

$$E - \frac{\hbar^2}{2M} \cdot \frac{N}{2} = \frac{\hbar^2}{2M} \cdot \frac{\epsilon}{2a} \qquad (4\text{-}32)$$

where ϵ is given in Table 4.1..

TABLE 4.1

	Exponential	Step
b	12.57	16.12
γ^{-1}	4.42	4.39
τ	2.92	0
α	5.24×10^3	5.24×10^3
δ	.222	.222
ε	2199.5	2235.4

A rather surprising result is that the step-function representation of the boson state increases the energy over the 'improved' wave-function (4-7) by only 1.6%. Thus for values of α (the coupling constant) such that $b > 10r_0$, the spherical well model for the ground state of the boson system is probably satisfactory.

For values of $b < 10r_0$, the slope of the boson wave-function becomes less as can be seen from the solutions for low α in Figure 3.2..

This region will be explored in section 4.3. where an estimate will be made of the minimum value of α showing bubble-like solutions. Here we will compare the energy (4-32) with the energy found by Burdick (1965) for an electron in a periodic lattice. The values of the parameters α and δ chosen above, were made with this comparison in mind.

The energy (4-32) is expressed in units of $r_0^{-2} = (8\pi a \rho)$. If values of a, ρ and M, that are relevant to liquid helium are used, we find $r_0 = .83\ \text{Å}$ and the value

$$E - \frac{4\pi a \rho N \hbar^2}{2M} = \cdot 324 \text{ eV} \qquad (4\text{-}33)$$

for the variational upper bound to the energy of the system. This should be compared with the energies $> 1 \cdot 0$ eV found by Burdick at approximately the same densities. The model used above is not applicable to densities as high as liquid helium densities, $(a^3\rho \approx \cdot 4)$, but the result suggest that probably the bubble represents a lower energy structure than a 'free' electron propagating through undisturbed He II. The difference between these energies is the binding energy of the bubble structure.

2. Excited Electronic States.

The simple spherical well model of the bubble gives rise to the following possibility. The depth of the well is

$$V_0 = \frac{2\pi l \hbar^2 \rho_0}{\mu} = \frac{\hbar^2}{2\mu} \cdot \frac{\delta}{2r_0^2} \qquad (4\text{-}34)$$

and the radius from Table 4.1. is

$$b = 16 \cdot 12\, r_0 \qquad (4\text{-}35)$$

From the simple quantum-mechanical theory of the spherical well, it is known that the well will support a p-state if

$$V_0 b^2 > \frac{\pi^2 \hbar^2}{2\mu} \qquad (4\text{-}36)$$

With (4-34), this condition becomes

$$b > \left(\frac{2\pi^2}{\delta}\right)^{1/2} r_0 = 9.43\, r_0 \qquad (4\text{-}37)$$

when $\delta = .222$. Hence since (4-35) satisfies this inequality, there exists an excited state of the electron that would still be trapped. Actually the radius of the bubble is sufficiently large to maintain a second s-state, but this is close to the top of the well and the curvature of the walls may increase the energy of the state beyond the well depth. It is straightforward (see for example Schiff, 1955) to calculate the energy difference between the ground state and the p-state. We find

$$E_p - E_{s_1} = 2.72 \times 10^{-2} \left(\frac{\hbar^2}{2\mu r_0^2}\right) \qquad (4\text{-}38)$$

and between the higher s-state and the ground state

$$E_{s_2} - E_{s_1} = 7{\cdot}04 \times 10^{-2} \left(\frac{\hbar^2}{2\mu r_0^2}\right) \tag{4-39}$$

If helium-densities are used to determine r_0 these differences are, ·150 eV and ·388 eV respectively. Thus, with radiation of about 21·0 μ wavelength it should be possible to excite the electron into its p-state. The boson system would then accomodate to the new electronic state by emitting phonons and the system would find a new self-consistent state, presumably with p-wave symmetry. This provides a method of testing the bubble theory for negative ions in liquid helium. The density of negative ions may be too low to permit seeing an absorption line but if the p-wave accomodated state decays to an s-state, it may be possible to see a line at a longer wavelength.

3. Least Value of the Coupling Constant.

The variational procedure used above, provides us with a means of estimating the least value of the coupling constant α that can sustain a bubble. That this minimum α exists, can be understood from the spherical well model used above. The radius of the well, b , is monotonically dependent on the coupling constant α . For small values of α , b decreases to a value at which the criterion

$$V_0 b^2 > \frac{\pi^2 \hbar^2}{8\mu} \qquad (4\text{-}40)$$

can no longer be satisfied and no bound states of the impurity exist. The penetration of the electronic wave-function into the boson system becomes so great that it becomes energetically favourable for the cavity to collapse and the electron to become a free particle in the medium. In reality, the transition from the bubble mode to the free-electron mode is governed by the relative energies of the two modes. Our optical model of helium cannot describe the free-electron mode at all so the calculation that follows at best, can only give an order of magnitude of the minimum value of α . This can be obtained from equations (4-16) and (4-18). Eliminating b from these equations we rapidly obtain

$$\frac{4\alpha}{7} = \left(\frac{3x^2}{\delta^3 G^3}\right)^{1/2}\left(\delta A + \frac{3x^2 B}{G}\right) \qquad (4\text{-}41)$$

where $A \equiv A(y)$, $B \equiv B(y)$ and $G \equiv G(x,y)$ are defined in (4-19),(4-20) and (4-24). Now the function of x and y on the right-hand side of (4-41) has a positive minimum. Hence in order to be able to minimise the energy of the system we must have that,

$$\frac{4\alpha}{7} \geqslant \min\left\{\left(\frac{3x^2}{\delta^3 G^3}\right)^{1/2}\left(\delta A + \frac{3x^2 B}{G}\right)\right\} \qquad (4\text{-}42)$$

$G(x,y)$ is a complicated function of x and y and no attempt has been made to find the exact values of x and y that minimise (4-42) and satisfy (4-17). However if $y \gg 1$, $x^2 G^{-3}$ has its minimum near $x = 1$ and also if $y \ll x$ $x^2 G^{-3}$ has its minimum near $x = 1$. Putting $x = 1$ in (4-42) and minimising with respect to y, we find the minimum occurs near $y = 4$ if $\delta = \cdot 222$, giving

$$\frac{4\alpha}{7} \gtrsim 75\cdot 0 \qquad (4\text{-}43)$$

However $y - 4\cdot 0$, $x = 1\cdot 0$ does not satisfy (4-17) hence does not represent a true minimum to the energy of the system. If $x = 1$, y can be determined from equation (4-25) for a given value of δ . The value $y = 1\cdot 4$ approximately satisfies the equations giving

$$\frac{4\alpha}{7} \geqslant 114$$

$$\text{or} \quad \alpha \geqslant 200 \qquad (4\text{-}44)$$

It is of interest to perform the same calculation using a step-function representation for the boson wave-function although we might expect this to be a bad representation because of the low value of y found above ($y = {}^{b}/_{\tau}$, where τ is essentially the width of the surface of the boson state). The calculation gives as a minimum for $(\alpha\,\delta^{3/2})$

$$\alpha\,\delta^{3/2} \gtrsim 21\cdot 6 \qquad (4\text{-}45)$$

or if $\delta = \cdot 222$,

$$\alpha \geqslant 216 \qquad (4\text{-}46)$$

Thus to obtain an order of magnitude the stepfunction is good enough.

Figure 3.2. shows how the computed solutions behave as α approaches these low values. Much below $\alpha = 500$, it became impossible even to approximately satisfy the boundary conditions, because as the lower end of the boson wave-function approached the origin, it diverged more and more rapidly. Thus it was found impossible to generate solutions for low values of α that still satisfied the integral condition on R_1 .

CHAPTER 5.

THE EFFECTIVE MASS.

In the preceding chapter we have dealt with the ground state of boson system in semi-classical manner. This can only be regarded as a first approximation to a quantum-mechanical treatment of the interacting bosons and impurity. In the case of strong coupling the disturbance of the ground state and the energy of the trapped impurity dominate the changes in the energy of the system. When the coupling is weak, so that disturbance of the ground state is neglegible, and in the intermediate coupling case (the transition region) interactions involving excited states of the boson system will become important. We will consider the latter two cases in the next chapter. Here, we will discuss mainly the strongly coupled impurity.

1. Excited Boson States in Strong Coupling.

The Hamiltonian covering all strengths of the coupling constant is

$$H = H_b + H_e + H_{be} \tag{5-1}$$

where

$$H_b = -\frac{\hbar^2}{2M}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i>j}\sum V\left(|\underline{x}_i - \underline{x}_j|\right) \tag{5-2}$$

$$H_e = -\frac{\hbar^2}{2\mu}\nabla_e^2 \tag{5-3}$$

$$H_{be} = \sum_{i=1}^{N} W\left(|\underline{y} - \underline{x}_i|\right) \tag{5-4}$$

To enable us to treat the excited states as well as the ground state of the bosons, we will transform from the Schrödinger representation to the formalism of second quantization for the bosons.

$$\begin{aligned} H_b &= -\frac{\hbar^2}{2M}\int \Psi^+_{(\underline{x})}\nabla^2\Psi_{(\underline{x})}\, d^3x \\ &\qquad + \frac{1}{2}\int \Psi^+_{(\underline{x}')}\Psi_{(\underline{x})} V\left(|\underline{x}-\underline{x}'|\right)\Psi_{(\underline{x})}\Psi_{(\underline{x}')}\, d^3_x\, d^3x' \\ H_e &= -\frac{\hbar^2}{2\mu}\nabla_y^2 \\ H_b &= \int \Psi^+(\underline{x})\, W\left(|\underline{x}-\underline{y}|\right)\Psi_{(\underline{x})}\, d^3x \end{aligned} \tag{5-5}$$

where $$\left[\Psi(\underline{x}), \Psi^{+}(\underline{x}') \right] = \delta(\underline{x} - \underline{x}') \qquad (5\text{-}6)$$

The Hamiltonian in this form has been studied by Gross (1962) for the weak-coupling case in which $W(|\underline{x} - \underline{y}|)$ is a hard-core plus a polarization potential and by Girardeau (1961) for the weakly coupled case when $W(|\underline{x} - \underline{y}|)$ is solely a repulsive hard-core. Gross (1958) also outlines the equations we have analysed in Chapters 3. and 4.. Writing the whole Hamiltonian in second quantization notation, we have

$$H_b = -\frac{\hbar^2}{2M} \int \Psi^{+}(\underline{x}) \nabla^2 \Psi(\underline{x})\, d^3x + \frac{1}{2} \int \Psi^{+}(\underline{x}') \Psi^{+}(\underline{x}) V(|\underline{x} - \underline{x}'|) \Psi(\underline{x}) \Psi(\underline{x}')\, d^3x\, d^3x'$$

$$H_e = -\frac{\hbar^2}{2\mu} \int \phi^{+} \nabla^2 \phi \, d^3y$$

$$H_{be} = \iint \phi^{+}(\underline{y}) \Psi^{+}(\underline{x}) W(|\underline{y} - \underline{x}|) \phi(\underline{y}) \Psi(\underline{x})\, d^3x\, d^3y \qquad (5\text{-}7)$$

This is the Hamiltonian of two interacting quantized fields. The operators $\phi(\underline{y})$, $\phi^{+}(\underline{y})$, if we are considering the impurity to be an electron, obey the anti-commutation relation

$$\left[\phi(\underline{y}), \phi^{+}(\underline{y}') \right]_{+} = \delta(\underline{y} - \underline{y}') \qquad (5\text{-}8)$$

We can simplify the Hamiltonian somewhat if we use the Bogolubov approximation and assume that a single boson state is macroscopically occupied and that no other state is so occupied. Expand in terms of an orthonormal basis $\eta_i(\underline{x})$, $i = 0, \dots \infty$.

$$\Psi(\underline{x}) = \sum_{n=0}^{\infty} b_n \eta_n(\underline{x})$$

$$\Psi^+(\underline{x}) = \sum_{n=0}^{\infty} b_n^+ \eta_n^*(\underline{x}) \qquad (5\text{-}9)$$

where $\Omega^{-1} \int |\eta_i(\underline{x})|^2 d^3x = 1$

and choose $\eta_0(\underline{x})$ to be the 'most-occupied' boson state. Here the b_n, b_n^+ are the creation and annihilation operators for particles into the states $\eta_n(\underline{x})$,

$$b_n = \frac{1}{\Omega^{1/2}} \int \Psi(\underline{x}) \eta_n^*(\underline{x})\, d^3\underline{x} \qquad (5\text{-}10)$$

We may extract the $\eta_0(\underline{x})$ state by writing

$$\Psi(\underline{x}) = \Psi_0(\underline{x}) + \Psi_{ex}(\underline{x}) \qquad (5\text{-}11)$$

in the Hamiltonian (5-7), where

$$\Psi_0(\underline{x}) = \frac{1}{\Omega^{1/2}} b_0 \eta_0(\underline{x}) \qquad (5\text{-}12)$$

and $\Psi_{ex}(\underline{x})$ represents the sum of other possible states available to the bosons

$$\Psi_{ex}(\underline{x}) = \frac{1}{\Omega^{1/2}} \sum_{n=1}^{\infty} b_n \, \eta_n(\underline{x}) \tag{5-13}$$

Writing (5-11) in (5-7) and extracting only the Ψ_0 dependent terms and the terms linear in Ψ_{ex}, we obtain

$$\begin{aligned} H_b = {} & \frac{\hbar^2}{2M} \int \nabla \Psi_0^+ \cdot \nabla \Psi_0 \, d^3x + \frac{1}{2} \int \Psi_0^+(x) \, \Psi_0^+(x') \, V(|\underline{x}-\underline{x}'|) \, \Psi_0 \Psi_0 \, d^3x \, d^3x' \\ & + \frac{\hbar^2}{2M} \int \left(\nabla \Psi_0^+ \cdot \nabla \Psi_{ex} + \nabla \Psi_{ex}^+ \cdot \nabla \Psi_0 \right) d^3x \; + \\ & \int \Psi_0^+ \Psi_0^+ \, V(|\underline{x}-\underline{x}'|) \, \Psi_0 \Psi_{ex} \, d^3x \, d^3x' + \int \Psi_0^+ \Psi_{ex}^+ \, V(|\underline{x}-\underline{x}'|) \, \Psi_0 \Psi_0 \, d^3x \, d^3x' \end{aligned} \tag{5-14}$$

$$H_e = \frac{\hbar^2}{2\mu} \int \nabla \phi^+ \cdot \nabla \phi \, d^3y \tag{5-15}$$

$$\begin{aligned} H_{be} = {} & \iint \phi^+(\underline{y}) \, \Psi_0^+(\underline{x}) \, W(|\underline{y}-\underline{x}|) \, \phi(\underline{y}) \, \Psi_0(\underline{x}) \, d^3x \, d^3y \\ & + \iint \phi^+ \, \Psi_0^+ \, W(|\underline{y}-\underline{x}|) \, \phi \, \Psi_{ex} \, d^3x \, d^3y \\ & + \iint \phi^+(\underline{y}) \, \Psi_{ex}^+ \, W(|\underline{y}-\underline{x}|) \, \phi \, \Psi_0 \, d^3x \, d^3y \end{aligned} \tag{5-16}$$

Now since the state $\eta_0(x)$ is macroscopically occupied we can, following Bogolubov, replace b_0 by $n_0^{1/2}$, so that

$$\Psi_0(x) = \left(\frac{n_0}{\Omega}\right)^{1/2} \eta_0(x) \tag{5-17}$$

If we assume that the electron is a single particle and occupies a given state, we can also replace the operator $\phi(\underline{x})$ by its equivalent state $\phi(\underline{x})$, and $\phi^+(x)$ by $\phi^*(x)$. Then putting $\Psi_{ex}(\underline{x}) = 0$, and using only the first lines of (5-14), (5-15) and (5-16), we have the Hamiltonian used in Chapter 3.. The analysis that followed showed that $\Psi_0(\underline{x})$ and $\phi(\underline{y})$ were given the computed curves in Figure 3.2.. The above approximation is equivalent to assuming that n_0, the ground state occupation number, equals N, the total number of particles, since the number operator is

$$\begin{aligned} N_{op} &= \int \Psi^+(x)\, \Psi(x)\, d^3x \\ &= n_0 + \int \left(\Psi_0^+(x)\, \Psi_{ex} + \Psi_{ex}^+\, \Psi_0 \right) d^3x + O(\Psi_{ex}^2) \end{aligned} \tag{5-18}$$

Hence putting $\Psi_{ex} = 0$, we have $n_0 = N$.

To improve on the lowest order result we need to include the oscillations of the boson s system about its lowest state $\Psi_0(\underline{x})$ that are concealed in $\Psi_{ex}(\underline{x})$. These excited states represent different configurations of the bosons, each of which presents to the electron a different array of potentials in which to move. We have already assumed that the electron can adiabatically follow the changing configuration of the bosons. In our variational treatment we have shown that only those configurations that produce a potential well in which the electron can reduce its energy are important. The electron energy is degenerate as the shape of the well can vary continuously but within a given well it exists in discrete states. Since these higher electronic states are separated from the lowest state by an energy of the same order as the depth of the well, we can probably ignore transitions of the electron into these states. The approximation is equivalent to the Born-Oppenheimer approximation in metals and is used in strong-coupling theories of the polaron, (see Allcock, 1956, for a review).

Since only a small number of bosons is not in the state Ψ_0 , the electronic wave-function is largely determined by the variational procedure. Thus as a first approximation to the self-energy of the bubble, we can take Ψ_0 and ϕ as determined by the variational ansatz. This procedure separates out the electronic part of the Hamiltonian and we are effectively left with the problem of a boson system bounded on the one hand, at a large distance, by the walls of the container and on the other by the surface of the bubble. The electron-boson interaction term in the Hamiltonian becomes a single-particle potential acting on the boson system if we assume $\phi(\underline{y})$ to be known and integrate over $\underline{y}$. Even if $W(|\underline{x}-\underline{y}|)$ is taken to be proportional to $\delta(|\underline{x}-\underline{y}|)$, the Dirac δ-function, the problem is still non-trivial because the electron density $\phi^*(\underline{y})\,\phi(\underline{y})$ at any $\underline{y}$ is not a simple function. Probably the simplest form of the problem that one might hope to treat analytically is to assume that the electronic bubble constitutes a hard-sphere in the boson system and force the boson wave-function to vanish on the surface of the sphere by using a pseudo-potential. One could expand the boson wave-function $\Psi(\underline{x})$ in terms of spherical harmonics and suitable radial wave-functions. This is essentially the method suggested by Gross (1962) in connection with the problem of the heavy impurity. Notice we have altered the light impurity problem to one with infinite mass as we have not permitted recoil of the bubble in any interaction with the excited boson states. This is not a too strong assumption as the effective mass of the bubble is indeed large. However distortions of the bubble may be important, and should be included in any attempt at analysis.

2. The Effective Mass.

Throughout the work, so far, we have formulated the problem as a static one without consideration of the possible motions of the electron through the bosons. In order to obtain the effective mass, we have to reformulate the problem in a way that permits us to obtain the energy E of the system as a function $E(p)$ of the total momentum $\underline{P}$.

Since the Hamiltonian (5-7) is translationally invariant, the total momentum is a constant of the motion. The total momentum operator $\underline{P}$ is

$$\underline{P} = -\frac{i\hbar}{2}\left[\int\left(\phi^{+}\nabla\phi - \nabla\phi^{+}\cdot\phi\right)d^3y + \int\left(\Psi^{+}\cdot\nabla\Psi - \nabla\Psi^{+}\cdot\Psi\right)d^3x\right] \tag{5-19}$$

which can readily be shown to satisfy

$$i\hbar\,\frac{d\underline{P}}{dt} = \left[\,\underline{P}\,,\,H\,\right] = 0 \tag{5-20}$$

In the Hartree approximation, we can replace the ϕ operator and the Ψ operator by the chosen occupied state wave-functions, and their Hermitean conjugates by the complex conjugate states. This leads us to the equation

$$\langle\underline{P}\rangle = -\frac{i\hbar}{2}\left[\int\left(\phi^{*}\nabla\phi - \nabla\phi^{*}\cdot\phi\right)d^3y + \int\left(\Psi_0^{*}\cdot\nabla\Psi_0 - \nabla\Psi_0^{*}\cdot\Psi_0\right)d^3x\right] \tag{5-21}$$

We should attempt to find wave-functions that diagonalize both $\underline{P}$ and H simultaneously. Clearly the Hartree wave-functions used previously can in no way do this. On the other hand it is reasonably to assume that at low momenta the bubble will not be greatly distorted and that the density distribution of bosons around the bubble is largely described by the stationary state density. This is equivalent to assuming the boson system is a nearly incompressible fluid and the problem of the effective mass of the bubble becomes hydrodynamical. If we assume that the bubble constitutes a hard-sphere and that there is a dipolar flow around it, the effective mass is

$$M_{eff} = \frac{1}{2}\left(\frac{4}{3}\pi b^3\right)\rho_\infty + \mu \qquad (5\text{-}22)$$

where ρ_∞ is the equilibrum boson density. This assumes that the density of the bosons is uniform up to the bubble surface and zero inside it, i.e. a step-function. We have seen variationally that this gives a good estimate of the energy despite the interpenetration of the two fields and hence (5-22) probably is a close approximation to the real effective mass. In any case, corrections to this estimate from quantum effects will almost certainly be smaller, in any application of the theory to the negative ion, than corrections due to polarization increases in the density around the ion. However the theory can be put on a more rigorous basis, by assuming a general wave-function that diagonalises $\underline{P}$ and performing a functional variation to minimise the expectation value of the Hamiltonian. This has been done for the heavy impurity by Feynman (1954) and for the heavy ion by Gross (1962) and we will apply much the same arguments to the light impurity here.

We do not wish to consider explicitly the momentum of the electron, only its average velocity through the bosons. Hence we need a description of the bubble which reduces to the Hartree state in the limit of zero velocity.

Because such a description cannot diagonalise the total momentum we need a different variational procedure from the usual one. We will use a method described by Allcock (1956) and applied by him to the effective mass of a polaron in the strong coupling limit. We describe the bubble by a wave packet and attempt to satisfy the time dependent Schrödinger equation. We will find a new variational principle that tells us whether our trial wave-functions are approximate solutions of this equation or not.

Consider the following time dependent wave-functions

$$\chi(\underline{q},t) = e^{-\frac{i}{\hbar}(\underline{P}\cdot\underline{V}+\lambda)t}\,\Psi(\underline{x}-\underline{q},\underline{x}_1-\underline{q},\dots\underline{x}_N-\underline{q}) \tag{5-23}$$

This represents a distribution of the bosons and the impurity about the point $\underline{q}$ which is moving through the liquid with velocity $\underline{V}$. In order that $\chi(\underline{q},t)$ represents a solution of the time dependent Schrödinger equation, Allcock suggests that $\chi(\underline{q},t)$ should be chosen to minimise the positive definite expression

$$S \equiv \left\langle \chi \middle| \left\{-i\hbar\overleftarrow{\frac{\partial}{\partial t}} - H\right\}\left\{i\hbar\frac{\partial}{\partial t} - H\right\} \middle| \chi \right\rangle \tag{5-24}$$

Minimising first with respect to λ, we find trivially that

$$\lambda = \langle \chi(q,0) | H - \underline{P}\cdot\underline{V} | \chi(q,0) \rangle$$

and that S reduces to

$$\langle \chi(q,0) | (H - \underline{P}\cdot\underline{V})^2 | \chi(q,0) \rangle - \left[\langle \chi(q,0) | H - \underline{P}\cdot\underline{V} | \chi(q,0) \rangle \right]^2 \tag{5-25}$$

Now Allcock points out that any eigenstate of the operator $H - \underline{P}\cdot\underline{V}$ will exactly minimise (5-25), and moreover the lowest will correspond to the lowest eigenstate of H. So we look for the lowest eigenstate of $(H - \underline{P}\cdot\underline{V})$, or equivalently minimise

$$J_{\underline{V}} = \langle \chi(q,0) | H - \underline{P}\cdot\underline{V} | \chi(q,0) \rangle \tag{5-26}$$

with $\langle \chi | \chi \rangle = 1$

To find the effective mass we observe (see Allcock, 1962) that if $\chi_{\underline{p}}$ is an eigenstate that diagonalises both H and $\underline{P}$ then

$$H \chi_{\underline{p}} = E(p)\, \chi_{\underline{p}} \tag{5-27}$$

and

$$\underline{P}\, \chi_{\underline{p}} = \underline{p}\, \chi_{\underline{p}} \tag{5-28}$$

where $\underline{p}$ is the momentum eigenvalue corresponding to the state $\chi_{\underline{p}}$. Also that for small $\underline{p}$

$$E(\underline{p}) = E(0) + \frac{p^2}{2M_{eff}} \tag{5-29}$$

where M_{eff} is defined as the effective mass. Hence the eigenvalues of $J_{\underline{V}}$ are

$$E(0) + \frac{p^2}{2M_{eff}} - \underline{p} \cdot \underline{V} \qquad (5\text{-}30)$$

which has a minimum at $\underline{p} = M_{eff} \underline{V}$,

$$E(0) - \frac{1}{2} M_{eff} V^2 \qquad (5\text{-}31)$$

Hence we can estimate M_{eff} from the formula.

$$\frac{1}{2} M_{eff} = \left[\frac{\min J_0 - \min J_{\underline{V}}}{V^2} \right]_{V \to 0} \qquad (5\text{-}32)$$

Now the function $\chi(q,0)$ must allow for the motion of the bubble and also a backflow of bosons around the bubble. On the other hand since as $V \to 0$ we expect the impurity to be in a Hartree state, let us write

$$\begin{aligned} \chi(q,0) &= \Psi(\underline{x} - \underline{q}, \underline{x}_i - \underline{q}) \\ &= e^{\frac{i\mu \underline{V} \cdot \underline{x}}{\hbar}} \phi(\underline{x} - \underline{q}) \prod_{i=1}^{N} f(\underline{x}_i - \underline{q}) e^{iS(\underline{x}_i - \underline{q})} \end{aligned}$$

$$(5\text{-}33)$$

Then the expectation value of $(H - \underline{P} \cdot \underline{V})$ is

$$J_{\underline{V}} = \Big[\frac{\hbar^2}{2\mu} \int (\nabla\phi)^2 d^3x + \frac{\hbar^2 N}{2M} \int (\nabla f)^2 d^3x$$
$$+ \frac{N(N-1)}{2} \int f^2(x) V(|\underline{x} - \underline{x}'|) f^2(x') \, d^3x \, d^3x'$$
$$+ N \int f^2(x) \, W(|\underline{x} - \underline{x}'|) \, \phi^2(x') \, d^3x \, d^3x' \Big]$$
$$+ \Big[-\frac{\mu V^2}{2} \int \phi^2 d^3x + \frac{\hbar^2 N}{2M} \int (\nabla s)^2 f^2 d^3x - \hbar \underline{V} N . \int \nabla s \, f^2 d^3x \Big]$$

(5-34)

Writing $\Psi^2 = N f^2$, we see that the first bracket in this expression is the term we minimised before. Also if $\int \phi^2 d^3x = 1$ then the second bracket becomes

$$\Delta J \equiv -\frac{\mu V^2}{2} + \frac{\hbar^2}{2M} \Big\{ \int (\nabla s)^2 \Psi^2 d^3x - 2\underline{k} . \int \nabla s \, \Psi^2 d^3x \Big\}$$

(5-35)

where we have written $\hbar \underline{k} = M \underline{V}$.

let us assume at this point that the backflow around the bubble may be described by a dipolar flow. i.e.

$$s(\underline{x}) = \frac{A z}{r^3}$$

(5-36)

where we take z along the direction of $\underline{V}$.

Following Feynman (1954), we have to slightly alter $S(\underline{x})$ at large distances so that the last term in (5-35) converges and may be integrated by parts. Then minimising with respect to A we find after a straightforward calculation

$$A = -\frac{k}{2}\left(\frac{4}{3}\pi\rho_\infty\right) I^{-1} \qquad (5\text{-}37)$$

and
$$\Delta J = -\frac{V^2}{2}\left[\mu + \frac{M}{2}\left(\frac{4}{3}\pi\rho_\infty\right) I^{-1}\right] \qquad (5\text{-}38)$$

where
$$I = \int_0^\infty \frac{\psi^2(r)}{r^6} \cdot 4\pi r^2 dr$$

To obtain this result we have assumed that $\psi^2(\underline{r})$ is a function of $|\underline{r}|$ only. In the notation of Feynman, $\psi^2(\underline{r}) = p(\underline{r})$.

It is unnecessary to minimise $J(\underline{v})$ with respect to ϕ and f for the following reason. $J(\underline{v})$ differs from J_0 only in order V^2. So if (ϕ_0, f_0) minimises J_0 and $(\phi_{\underline{v}}, f_{\underline{v}})$ minimises $J_{\underline{v}}$, then $(\phi_0, f_0) - (\phi_{\underline{v}}, f_{\underline{v}})$ will be of order V^2. For the difference between J_v and J_0 can be regarded as a small perturbation of J_0 and the perturbation of the wave-function will be of the same order. We have also

$$J_{\underline{V}} = J_0 + \Delta J \tag{5-39}$$

and since (ϕ_0, f_0) minimises J_0, then $J_0(\phi_v, f_v) - J_0(\phi_0, f_0)$ is of order $[(\phi_v, f_v) - (\phi_0, f_0)]^2$, i.e. of order V^4. Hence using ϕ_0 and f_0 in $J_{\underline{V}}$ in place of $(\phi_{\underline{V}}, f_{\underline{V}})$ only introduces terms of order V^4. So to determine the effective mass we may use our previously found value of Ψ^2.

Hence

$$M_{eff} = \mu + \frac{M}{2}\left(\frac{4}{3}\pi\rho_\infty\right)^2 \left[\int_0^\infty \frac{\Psi^2_{(r)}}{r^6} \cdot 4\pi r^2 dr\right]^{-1} \tag{5-40}$$

The step-function ansatz for $\Psi_{(\underline{r})}$ gives the hydrodynamical mass (5-22). Using the $\Psi_{(\underline{r})}$ found in Chapter 3. slightly reduces the effective mass but we have not undertaken this calculation as (5-40) neglects the important polarization induced mass. Gross (1962) has pointed out that around the positive ion one no longer gets dipolar flow if one includes the attractive polarization forces. The procedure he adopts will be outlined below.

The polarization effect, which is dominant in the positive ion case, is not so important in the negative ion case, because the region immediately around the charge is cleared of bosons. The polarization force rapidly falls off (as r^{-5}) and is small outside the bubble radius. However Kuper finds that it increases the effective mass even of the negative ion by 20%. Notice, that because of the spherical symmetry of the bubble and the fact that the electron is largely localised we can consider the charge as located at the bubble centre. Actually the bosons experience a rapidly fluctuating force as the electron oscillates across the bubble but the frequency of this fluctuation is so large that the bosons cannot respond to the force. The frequency ω_e of the fluctuation is of the order of $\hbar/2\mu b^2$, whereas the natural frequency of the bosons is $\omega_b = \hbar/2m r_0^2$. Since

$$\frac{b^2}{r_0^2} \ll \frac{M}{\mu} \tag{5-41}$$

we see that $\omega_e \gg \omega_b$.

To find a better $s(\underline{x})$ than dipolar, we use the variational principle on $S(\underline{x})$. In our case this leads to the equation,

$$\nabla . \left[p(r) \left(\underline{k} - \nabla s \right) \right] = 0 \qquad (5\text{-}42)$$

(cf. Feynman, 1954, equation 7-4. and Gross, 1962, equation 2-9.). Multiplying by $S(\underline{x})$, integrating and substituting back in ΔJ gives

$$M_{eff} = \mu + \beta M \qquad (5\text{-}43)$$

where β is defined by

$$\beta \underline{k} = - \int s \, \nabla p \; d^3 x \qquad (5\text{-}44)$$

Writing $S(\underline{r}) = kz \left(1 - \frac{v(r)}{r} \right)$ and inserting in (5-42) gives

$$\frac{d}{dr} \left(r^2 \, p(r) \, \frac{dv}{dr} \right) = 2 p v \qquad (5\text{-}45)$$

and in (5-44) gives

$$M_{eff} = \mu + M \left[4\pi B \rho_\infty + 4\pi \int_b^\infty (p - \rho_\infty) \, r^2 dr \right] \qquad (5\text{-}46)$$

where B is defined by the asymptotic form of

$V(r)$, $V(r) \sim r + B r^{-2}$, and b is the radius of the bubble, $\left.\frac{dv}{dr}\right|_{r=b} = 0$.

Gross solves (5-45) for the case $p(r) = K r^{-4}$, $b < r < c$; $p(r) = \rho_\infty$, $r > c$, and calculates the effective mass in terms of two parameters (1) the radius of the hard-core of the ion $r = b$ and (2) the radius $r = c$ at which $K r^{-4} = \rho_\infty$. He finds in the limit $b \ll c$

$$M_{eff} = \mu + \frac{\mu M}{\mu + M}\left[4\pi c^3 \rho_\infty \cdot \frac{c}{b}\right] \quad (5\text{-}47)$$

However his $p(r)$ is not applicable to the bubble as the polarization part is already small at the bubble radius. The best way to find the effective mass, including polarization, would be to minimise $J_{\underline{v}}$ with a polarization term included and solve for $V(r)$ from (5-45) numerically. This has not yet been undertaken.

CHAPTER 6.

THE WEAKLY COUPLED IMPURITY.

1. Introduction.

The weak-coupling case that we will consider in this chapter, covers a number of different physical situations. The coupling constant α depends not only on the relative masses of the impurity and the bosons, but also on the boson-impurity scattering length and on the density of the boson system. By 'weak-coupling' we shall mean that the impurity nearly leaves the bosons undisturbed, that is, that the ground state may be regarded as a uniform state. This criterion distinguishes this range of α from the strong coupling range where the boson ground state is greatly distorted.

Girardeau (1961) has treated the weak-coupling case of the heavy impurity. He restricts himself to heavy impurities by neglecting certain terms of order $\frac{m}{\mu}$ in his transformed Hamiltonian. Since the weak-coupling case also includes the light impurity in a low-density medium, we should be able to extend his work to cover the light impurity provided the coupling constant is sufficiently low.

2. The Polaron-Like Hamiltonian.

The Hamiltonian we shall use has been given in equation (5-5) and is, with the boson operators expressed in the notation of second quantization but with the impurity operators in the Schrödinger picture

$$\begin{aligned}
H &= H_b + H_e + H_{be} \\
H_b &= -\frac{\hbar^2}{2m} \int \Psi^+(\underline{x})\, \nabla^2 \Psi(\underline{x})\, d^3x \\
&\quad + \frac{1}{2} \int \Psi^+(\underline{x})\, \Psi^+(x')\, V(|\underline{x}-\underline{x}'|)\, \Psi(\underline{x}')\, \Psi(\underline{x})\, d^3x\, d^3\underline{x}' \\
H_e &= \frac{p^2}{2\mu} = -\frac{\hbar^2}{2\mu} \nabla_y^2 \\
H_{be} &= \int \Psi^+(\underline{x})\, W(|\underline{x}-\underline{y}|)\, \Psi(\underline{x})\, d^3\underline{x}
\end{aligned}$$

(6-1)

Since we have postulated that the ground state is undisturbed, let us follow the usual procedure and expand $\Psi(\underline{x})$ in plane-wave states

$$\Psi(\underline{x}) = \sum_{\underline{k}} b_{\underline{k}}\, \eta_{\underline{k}}(\underline{x}) = \frac{1}{\sqrt{\Omega}} \sum b_{\underline{k}}\, e^{i\underline{k}\cdot\underline{x}} \tag{6-2}$$

Denoting the boson creation and annihilation operators by $b_{\underline{k}}^{+}$ and $b_{\underline{k}}$ we obtain

$$H_b = \frac{\hbar^2}{2m} \sum_{\underline{k}} k^2 b_{\underline{k}}^{+} b_{\underline{k}} + \frac{1}{2\Omega} \sum_{\underline{k},\underline{\ell},\underline{m}} V_{\underline{k}}\, b^{+}_{\underline{\ell}+\underline{k}}\, b^{+}_{\underline{m}-\underline{k}}\, b_{\underline{m}}\, b_{\underline{k}}$$

$$H_e = \frac{p^2}{2\mu}$$

$$H_{be} = \frac{1}{\Omega} \sum_{\underline{k},\underline{\ell}} b^{+}_{\underline{\ell}-\underline{k}}\, W_{\underline{k}}\, b_{\underline{\ell}}\, e^{i\underline{k}\cdot\underline{y}} \tag{6-3}$$

where

$$V_{\underline{k}} = \int V(\underline{r})\, e^{-i\underline{k}\cdot\underline{r}}\, d^3\underline{r}$$

$$W_{\underline{k}} = \int W(\underline{r})\, e^{-i\underline{k}\cdot\underline{r}}\, d^3 r \tag{6-4}$$

The operators $b_{\underline{k}}$, $b_{\underline{k}}^{+}$ satisfy the commutation relations

$$\left[b_{\underline{k}}, b_{\underline{k}'}\right] = \left[b_{\underline{k}}^{+}, b_{\underline{k}'}^{+}\right] = 0$$

$$\left[b_{\underline{k}}, b_{\underline{k}'}^{+}\right] = \delta_{\underline{k},\underline{k}'} \tag{6-5}$$

and the total number operator $N = \sum_{\underline{k}} n_{\underline{k}} = \sum_{\underline{k}} b_{\underline{k}}^{+} b_{\underline{k}}$.

We have imposed periodic boundary conditions so that $\underline{k}$ takes discrete values. The $b_{\underline{k}}$ operators, of course, commute with $\underline{r}$ and $\underline{p}$ which obey the usual commutation relations for conjugate Schrödinger operators.

$$\left[r_i , p_j \right] = i\hbar \delta_{ij} \tag{6-6}$$

From the Hamiltonian (6-3), we separate out the $\underline{k} = 0$ state following the usual Bogolubov procedure (Bogolubov, 1947), and let $b_0 = n_0^{1/2}$, i.e. adopt the viewpoint that $n_0 \gg 1$ or any other $n_{\underline{k}}$. Replacing b_0 and b_0^{+} by $n_0^{1/2}$ only introduces an error of order n_0^{-1}. If we consider only those terms in the interaction part of H_b that have at least two factors $n_0^{1/2}$ and in H_{be} at least one, we obtain from (6-3)

$$\begin{aligned} H_b - \mu N = & \sum_{\underline{k} \neq 0} \left(\frac{\hbar^2 k^2}{2m} + \frac{V_0 n_0}{\Omega} + \frac{V_k n_0}{\Omega} - \mu \right) b_{\underline{k}}^{+} b_{\underline{k}} \\ & + \frac{n_0^2}{2\Omega} V_0 - \mu n_0 \\ & + \frac{n_0}{2\Omega} \sum_{k \neq 0} V_{\underline{k}} \left(b_{-\underline{k}}^{+} b_{\underline{k}}^{+} + b_{-\underline{k}} b_{\underline{k}} \right) \end{aligned}$$

$$H_e = \frac{\underline{p}^2}{2\mu}$$

$$H_{be} = \frac{n_0 W_0}{\Omega} + \frac{n_0^{1/2}}{\Omega} \sum_{\underline{k} \neq 0} W_{\underline{k}} \left(b_{\underline{k}}^{+} e^{-i\underline{k}\cdot\underline{y}} + b_{\underline{k}} e^{i\underline{k}\cdot\underline{y}} \right) \qquad (6\text{-}4)$$

where, following Hugenholtz and Pines (1959), we consider $H - \mu N$ in order to permit us to consider processes that do not conserve the total number of bosons N.

The next step is to diagonalise H_b. This we do by writing

$$a_{\underline{k}} = \lambda_k b_{\underline{k}} + \mu_k b_{-\underline{k}}^{+}$$

$$a_{\underline{k}}^{+} = \lambda_k b_{\underline{k}}^{+} + \mu_k b_{-\underline{k}} \qquad (6\text{-}5)$$

where λ_k and μ_k are c-numbers which are to be determined by the criterion that the terms involving $a_{\underline{k}}^{+} a_{-\underline{k}}^{+}$ and $a_{-\underline{k}} a_{\underline{k}}$ vanish in the transformed Hamiltonian. In order that the $a_{\underline{k}}$ obey the same commutation relations as the operators we choose

$$\lambda_k^2 - \mu_k^2 = 1 \qquad (6\text{-}6)$$

Thence, writing

$$\alpha_k = \left(\frac{\hbar^2 k^2}{2M} - \mu + \frac{V_0 n_0}{\Omega} + \frac{V_k n_0}{\Omega} \right)$$

and

$$E_k = \left[\alpha_k^2 - \frac{n_0^2 V_k^2}{\Omega^2} \right]^{1/2} \qquad (6\text{-}7)$$

we obtain

$$H_b = \frac{n_0^2 V_0}{2\Omega} + \sum_{k \neq 0} \left(E_k a_{\underline{k}}^+ a_{\underline{k}} + \tfrac{1}{2}\left(E_k - \alpha_k\right)\right)$$

$$H_e = p^2/2\mu$$

$$H_{be} = \frac{n_0 W_0}{\Omega} + \frac{n_0^{1/2}}{\Omega} \sum_{k \neq 0} \left(\frac{\hbar^2 k^2}{2mE_k}\right)^{1/2} W_k \left\{ a_{\underline{k}}^+ e^{-i\underline{k}.\underline{r}} + a_{\underline{k}} e^{i\underline{k}.\underline{r}} \right\} \qquad (6\text{-}8)$$

The values of λ_k and μ_k that give (6-7) are found from equation (6-6) together with

$$\left(\lambda_k^2 + \mu_k^2\right) \frac{2V_k n_0}{\Omega} = \alpha_k \lambda_k \mu_k \qquad (6\text{-}9)$$

Now the factor $\left(\hbar^2 k^2/2mE_k\right)$ is related by the Feynman-Bijl formula to $S(\underline{k})$. It has, in fact, been shown by Miller, Pines and Nozieres (1962) in the Bogolubov approximation to be exactly equal to $\frac{N}{n_0} S(\underline{k})$, where $S(\underline{k})$ is the liquid structure factor defined by

$$S(\underline{k}) = \frac{1}{N} \langle 0 | \rho_{\underline{k}} \rho_{\underline{k}}^+ | 0 \rangle = \int d^3r \; p(\underline{r}) e^{-i\underline{k}.\underline{r}} \qquad (6\text{-}10)$$

and $p(\underline{r}) = \frac{1}{N}\langle 0|\rho^{+}(0)\rho(r)|0\rangle$ is the pair correlation function. Hence we can write the Hamiltonian

$$H = E_0 + \frac{p^2}{2\mu} + \sum_{k\neq 0} E_k a^{+}_{\underline{k}} a_{\underline{k}} + \frac{N^{1/2}}{\Omega}\sum_{k\neq 0}(S_k)^{1/2} W_k \left\{ a^{+}_{\underline{k}} e^{-i\underline{k}\cdot\underline{r}} + a_{\underline{k}} e^{i\underline{k}\cdot\underline{r}} \right\} \tag{6-11}$$

where

$$E_0 = \frac{n_0^2 V_0}{2\Omega} + \frac{n_0^2 W_0}{\Omega} + \frac{1}{2}\sum_{k\neq 0}(E_k - \alpha_k) - \mu n_0 \tag{6-12}$$

Now expression (6-11) is a Hamiltonian of the type proposed by Fröhlich for the polaron problem (see Fröhlich, 1954). This Hamiltonian has been treated in a very elegant way by Feynman (1955) using his path integral techniques (Feynman, 1948), and it would be interesting to apply the same method to (6-11).

Feynman's treatment of the polaron problem covers all values of the coupling constant but this we can clearly not expect in this problem for the following reason. As we hwve seen in earlier chapters the strong coupling region corresponds to a macroscopic depletion of the uniform ground state. In setting up the Hamiltonian (6-11) we have assumed that everywhere n_o the number of particles in the ground state is large. Hence we cannot expect to find (6-11) describing the strictly localised impurity that exists in a density depression of the same order as the uniform density of the bosons. The theory should describe the weak-coupling and intermediate coupling regions where we can describe the density fluctuations around the impurity as a cloud of virtual excitations. Indeed the impurity particle has been so described by Girardeau (1961) and by Miller, Pines and Nozières (1962), using, in the former case, the intermediate coupling polaron technique of canonical transformations (Lee, Low and Pines, 1953) and in the latter case, perturbation theory. At least Feynman's method should reproduce the results of these works and, at best, may indicate the limits of validity of the Hamiltonian (6-11).

3. Path-Integral Methods.

Since (6-11), apart from the term E_c , is exactly of the general form given by Feynman in his paper (1955, the last two equations are the relevant ones here) we can immediately write down the energy intergral that has to be minimised with respect to the parameters used by Feynman in his trial action :

$$\Delta E = \frac{3}{4v}(v-\omega)^2 - \iint_0^\infty \exp\left[-E_k\tau - \frac{k^2}{2}\frac{F(\tau)}{v^2}\right]\rho S_k W_k^2\, d\tau \frac{d^3k}{(2\pi)^3} \tag{6-13}$$

where $F(\tau) = \omega^2\tau + \frac{v^2-\omega^2}{v}\left(1-e^{-v\tau}\right)$; $\rho = \frac{N}{\Omega}$;
v , ω are the variational parameters, and we have taken $\hbar = \mu = 1$ in accord with Feynman. To establish contact with earlier work, we can let $v = \omega$, in which case the energy should correspond to that found by the perturbation theory method, since this is equivalent to taking as the trial action

$$S_1 = -\frac{1}{2}\int\left(\frac{d\underline{x}}{dt}\right)^2 dt \tag{6-14}$$

i.e. the action of a free particle. We have used here Feynman's notation, i.e. t stands for it'

where t' is real time and S_1 stands for iS' where S' corresponds to the more commonly defined action.

When $V = \omega$

$$\frac{1}{V^2} F(\tau) = \tau \qquad (6\text{-}15)$$

and integrating over τ gives

$$\Delta E_{V=\omega} = -\frac{\rho}{(2\pi)^3} \int_0^\infty \frac{S_k W_k^2 \, d^3k}{\left(E_k + \frac{k^2}{2}\right)} \qquad (6\text{-}16)$$

Substituting for S_k from (6-7) and using the result that the chemical potential $\mu = \frac{N_0 V_0}{\Omega}$, we obtain

$$\Delta E_{V=\omega} = -\frac{\rho}{(2\pi)^3} \int_0^\infty \frac{k^2 W_k^2 \, d^3k}{2mE_k \left[E_k + \frac{k^2}{2} \right]} \qquad (6\text{-}17)$$

where $$E_k = \frac{k}{2m} \left(k^2 + 4m\rho_0 V_k \right)^{1/2} \qquad (6\text{-}18)$$

Now (6-17) is exactly the perturbation theory result with the total momentum $\underline{P} = 0$, found by Miller, Pines and Nozières. As expected, Feynman's theory reproduces this result. The same thing can be shown for the effective mass. We are however interested in going beyond perturbation theory and would like to be able to integrate (6-13) for values of v and ω other than $v = \omega$. Let us look, following Feynman, at the case $v = (1+\varepsilon)\omega$ where ε is small. Then, to first order in ε,

$$\frac{1}{v^2} F(\tau) = \tau + \frac{2\varepsilon}{\omega}\left(1 - \omega\tau - e^{-\omega\tau}\right) \tag{6-19}$$

and ΔE becomes

$$\begin{aligned}\Delta E_\varepsilon &= \Delta E_{v=\omega} + \frac{3}{4}\varepsilon^2\omega \\ &\quad + \iint_0^\infty \exp\left[-\left(E_k + \frac{k^2}{2}\right)\tau\right] \frac{k^2\varepsilon}{\omega}\left(1-\omega\tau-e^{-\omega\tau}\right)\rho S_k W_k^2 \frac{d\tau\, d^3k}{(2\pi)^3} \\ &= \Delta E_{v=\omega} + \frac{3}{4}\varepsilon^2\omega - \frac{\varepsilon\omega\rho}{2\pi^2}\int_0^\infty \frac{S_k W_k^2 k^4 dk}{\left(E_k+\frac{k^2}{2}\right)^2\left(E_k+\frac{k^2}{2}+\omega\right)}\end{aligned} \tag{6-20}$$

We have, in order to proceed further, to assume a form of the potentials $W(|\underline{x}-\underline{y}|)$ and $V(|\underline{x}-\underline{x}'|)$. Since we are interested in the case of a hard-sphere impurity interacting with hard-sphere bosons we will use the pseudo-potentials already used in Chapter 3.,

$$V\left(|\underline{x}-\underline{x}'|\right) = \frac{8\pi a \hbar^2}{2M}\,\delta\left(\underline{x}-\underline{x}'\right) \qquad (3\text{-}18)$$

$$W\left(|\underline{x}-\underline{y}|\right) = \frac{8\pi \ell \hbar^2}{4\mu}\,\delta\left(\underline{x}-\underline{y}\right) \qquad (3\text{-}19)$$

These gives from (6-4)

$$V_k = \frac{4\pi a \hbar^2}{M} \qquad (6\text{-}21)$$

and

$$W_k = \frac{2\pi \ell \hbar^2}{\mu} \qquad (6\text{-}22)$$

4. The Perturbation Energy.

If we insert these forms of V_k and W_k in (6-20) and make no further comment, we would be neglecting an important point. The use of (6-21) for V_k need not worry us as we are only using the excitation spectrum of the bosons in (6-20) - the ground state energy having already been substracted off. However inserting (6-22) into the term $\Delta E_{V=\omega}$ i.e. (6-17), causes it to diverge. This is because (3-19) is not the correct pseudo-potential and fails when the wave-function on which it acts has a $1/r$ singularity at $r = 0$. A number of authors have proposed alterations of the original pseudo-potential treatment of Huang and Yang (1957), (notably Wu, 1959, Lieb, 1960, and Liu and Wong, 1963) that by various devices are arranged to remove the divergent terms automatically. However none is simpler to use in our case than the original method of Huang and Yang. This method consists of calculating the first order perturbation correction to the wave-function explicitly, so that the terms that have to be substracted out become obvious.

The first order correction to the ground state wave-function is from Miller, Pines and Nozières, (1962),

$$\psi^{(1)} = i \sum_{j=1}^{N} g(\underline{r}_j - \underline{R}) \, \phi_0 \, e^{i \underline{P} \cdot \underline{R}} \tag{6-23}$$

where $$g(\underline{r}) = \frac{i}{\Omega} \sum_{\underline{k}} \frac{W_{\underline{k}} \, e^{i \underline{k} \cdot \underline{r}}}{\left[E_{\underline{k}} + \frac{k^2}{2} - \underline{k} \cdot \underline{P} \right]} \tag{6-24}$$

We have to study $g(\underline{r})$, when $\underline{P} = 0$, near $r = 0$. Since $W_{\underline{k}}$ in (6-24) acts on a well-behaved function at $r = 0$ i.e. without a r^{-1} singularity, we can substitute from (6-22). Hence we need to look at the behaviour as $r \to 0$ of

$$g(\underline{r}) = 2\pi i \ell \sum_{\underline{k}} \frac{e^{i\underline{k}\cdot\underline{r}}}{\frac{k}{2m}(k^2+c^2)^{1/2} + \frac{k^2}{2}}$$

(6-25)

where $c^2 = (16\pi a \rho_0)$, and the sum is over all $\underline{k}$ of the form $\underline{k} = 2\pi(\ell, m, n)/L$ where $L^3 = \Omega$ and ℓ, m, n are integral and not all zero.

Taking the limit as $L \to \infty$, we can replace the summation by an integral

$$g(\underline{r}) = 2\pi i \ell \cdot \frac{1}{(2\pi)^3} \int d^3\underline{k} \; \frac{e^{i\underline{k}\cdot\underline{r}}}{\frac{k}{2m}(k^2+c^2)^{1/2} + \frac{k^2}{2}}$$

(6-26)

$$= \frac{2i\ell M}{\pi r} \int_0^\infty \frac{\sin kr \, dk}{Mk + (k^2+c^2)^{1/2}}$$

(6-27)

where we have extended the range of integration to $k = 0$ since this causes no singularity in the integral. The integral is a Fourier sine transform that in general cannot be done in closed form. However two special cases $M = 0$ and $M = 1$ can be done and are tabulated (Oberhettinger, 1957)

$$\int_0^\infty \frac{\sin kr}{(k^2+c^2)^{1/2}} = \frac{1}{2}\pi\left[I_0(cr) - \mathbb{L}_0(cr)\right] \tag{6-28}$$

$$\int_0^\infty \frac{\sin kr}{k + (k^2+c^2)^{1/2}} = \frac{1}{2}\frac{\pi}{cr}\left[I_1(cr) - \mathbb{L}_1(cr)\right] \tag{6-29}$$

where $I_\nu(z)$ is the modified Bessel function and $\mathbb{L}_\nu(z)$ is the modified Struve function. Since for small r, these functions behave as :

$$I_\nu(z) = \left(\frac{z}{2}\right)^\nu\left[\frac{1}{\Gamma(\nu+1)} + \frac{\left(\frac{z}{2}\right)^2}{1!\,\Gamma(\nu+2)} + \cdots\right] \tag{6-30}$$

$$\mathbb{L}_\nu(z) = \left(\frac{z}{2}\right)^{\nu+1}\left[\frac{1}{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\nu+\frac{3}{2}\right)} + \frac{\left(\frac{z}{2}\right)^2}{\Gamma\left(\frac{5}{2}\right)\Gamma\left(\nu+\frac{5}{2}\right)} + \cdots\right] \tag{6-31}$$

we see that as $r \to 0$, in the two cases,

$$\lim_{r\to 0} g(r)_{M=0} = i\ell M\left(\frac{1}{r} - \frac{2c}{\pi}\right) \tag{6-32}$$

$$\lim_{r\to 0} g(r)_{M=1} = \frac{i\ell}{2}\left(\frac{1}{r} - \frac{4c}{3\pi}\right) , \tag{6-33}$$

both of which contain a r^{-1} singularity.

The range of M that we are particularly interested in, is $M \gg 1$ i.e. small impurity mass. In this region we can evaluate the integral in (6-27) approximately in the following way.

Since the term Mk dominates the denominator for all $k > M^{-1}$, we can split the range of integration at $k = c$;

$$\int_0^\infty \frac{\sin kr \, dk}{Mk + (k^2+c^2)^{1/2}} = \int_0^1 \frac{\sin crt \, dt}{Mt + (t^2+1)^{1/2}} + \int_1^\infty \frac{\sin crt \, dt.}{Mt + (t^2+1)^{1/2}} \tag{6-34}$$

Since M is large and since the first integral converges as we go to the limit $r \to 0$,

$$\lim_{r\to 0}\int_0^\infty \frac{\sin kr\,dk}{Mk+(k^2+c^2)^{1/2}}$$

$$= \lim_{r\to 0}\left\{\int_1^\infty \frac{\sin crt\,dt}{(M+1)t}\left[1-\left(\frac{t-(t^2+1)^{1/2}}{(M+1)t}\right)+\left(\frac{t-(t^2+1)^{1/2}}{(M+1)t}\right)^2+O\left(\frac{1}{M^3}\right)\right]\right.$$

$$\left.+\int_0^1 \frac{crt\,dt}{Mt+(t^2+1)^{1/2}}+O(r^2)\right\}$$

$$= \lim_{r\to 0}\left\{-\frac{1}{(M+1)}si(cr)-\frac{cr}{(M+1)^2}\int_1^\infty\frac{dt}{t}\left(t-(t^2+1)^{1/2}\right)+\int_0^1\frac{crt\,dt}{Mt+(t^2+1)^{1/2}}+O\left(\frac{r}{M^3}\right)\right\} \tag{6-35}$$

Now both the remaining integrals can be done exactly by substituting $t=\frac{1}{2}\left(x-\frac{1}{x}\right)$ which reduces the integrands to rational functions.

$$\int_1^\infty\frac{dt}{t}\left(t-(t^2+1)^{1/2}\right) = -\int_{1+\sqrt{2}}^\infty \frac{x^2+1}{x^2(x^2-1)}\,dx$$

$$= \frac{1}{(1+\sqrt{2})}+\log\frac{1}{(1+\sqrt{2})} \tag{6-36}$$

$$\int_0^1\frac{t\,dt}{Mt+(t^2+1)^{1/2}} = \frac{1}{2(M+1)}\int_1^{1+\sqrt{2}}\frac{x^4-1}{x^2(x^2-\alpha^2)}\,dx$$

$$= \frac{1}{2(M+1)}\left[\sqrt{2}\left(1+\frac{1}{\alpha^2(1+\sqrt{2})}\right)+\frac{\alpha^4-1}{2\alpha^3}\ln\left(\frac{1-\alpha^2+\sqrt{2}(1+\alpha)}{1-\alpha^2+\sqrt{2}(1-\alpha)}\right)\right] \tag{6-37}$$

where $\alpha^2=\dfrac{M-1}{M+1}$.

Since as $r \to 0$

$$-\mathrm{si}\,(cr) \to \frac{\pi}{2} - cr + O(cr)^3 \qquad (6\text{-}38)$$

we have for large M ;

$$\lim_{r \to 0} g(r)_{M \gg 1} = i\ell \left\{ \frac{M}{(M+1)r} - \frac{2cM}{\pi(M+1)^2} \left[\ln \frac{2M}{(1+\sqrt{2})^2} - \frac{\sqrt{2}-1}{\sqrt{2}+1} \right] \right\} \qquad (6\text{-}39)$$

where the next term is of order M^{-2} . Thus in all the cases considered, we have an r^{-1} divergence plus a constant term. Denoting the constant in the brackets by $-\frac{2c}{\pi} f(M)$, we have for $\Delta E_{V=\omega}$ after removing the divergence,

$$\begin{aligned} \Delta E_{V=\omega} &= 2\pi\ell \cdot \frac{2c\ell}{\pi} f(M) \cdot \frac{N}{\Omega} \\ &= 4\pi^{1/2} \ell^2 (ap_0)^{1/2} \rho\, f(M) \end{aligned} \qquad (6\text{-}40)$$

where

$$\begin{aligned} f(M) &\sim M \qquad ; M \ll 1 \\ &= 1/3 \qquad ; M = 1 \\ &\sim \frac{M}{(M+1)^2} \left[\ln \frac{2M}{(1+\sqrt{2})^2} - \frac{\sqrt{2}-1}{\sqrt{2}+1} \right] \quad ; M \gg 1 \end{aligned} \qquad (6\text{-}41)$$

5. Higher Order Terms in the Energy.

As we have seen in equation (6-20) corrections to the total energy are of the form

$$\Delta E_{\varepsilon} = \frac{3}{4}\varepsilon^2\omega - \frac{\varepsilon\omega\rho}{2\pi^2}\int_0^\infty \frac{S_k W_k^2 k^4 dk}{\left(E_k + \frac{k^2}{2}\right)^2\left(E_k + \frac{k^2}{2} + \omega\right)} \tag{6-42}$$

Substituting for V_k, W_k, S_k and E_k from equation (6-21), (6-22), (6-7) and (6-18) and remembering that $\hbar = \mu = 1$, we can write (6-42) as

$$\Delta E_{\varepsilon} = \frac{3}{4}\varepsilon^2\omega - \frac{\varepsilon\omega\rho}{2\pi^2}\cdot 32M^3\pi^2\ell^2 \cdot \int_0^\infty k^3 dk \left\{(k^2+c^2)^{1/2}\left[(k^2+c^2)^{1/2} + Mk\right]^2\left[k(k^2+c^2)^{1/2} + Mk^2 + 2M\omega\right]\right\}^{-1} \tag{6-43}$$

where $c^2 = 16\pi a\rho_0$.

The integral can be done exactly. Writing $k = \frac{c}{2}\left(\frac{1}{x} - x\right)$ reduces the integral in (6-43) to

$$\frac{2}{(1+M)^3 c} I(\omega) \equiv \frac{2}{(1+M)^3 c}\int_0^1 \frac{(1-x^2)^3 dx}{(1-\alpha^2x^2)^2\left[(1-x^2)(1-\alpha^2x^2) + \frac{4\omega}{c^2}(1+\alpha^2)x^2\right]} \tag{6-44}$$

where again $\alpha^2 = \dfrac{M-1}{M+1}$.

Although (6-44) can in principle be evaluated exactly the expression obtained is complicated and not very illuminating, The expression (6-43) still has to be minimised with respect to ω and ε and in general this involves solving a transcendental equation. An interesting special case is obtained by letting $c = 0$ in equation (6-43) i.e. taking the boson spectrum to be proportional to k^2 instead of the Bogolubov spectrum. Then (6-43) reduces to

$$\Delta E_{\varepsilon} = \frac{3}{4}\varepsilon^2\omega - \frac{16 M^3 \ell^2 \rho}{(M+1)^3} \cdot \left(\frac{M+1}{2M}\right)^{1/2} \varepsilon\,\omega^{1/2} \cdot \frac{\pi}{2} \qquad (6\text{-}45)$$

which is a function of $(\varepsilon^2\omega)^{1/2}$ only and minimises when

$$\varepsilon\,\omega^{1/2} = \frac{2}{3} \cdot \frac{8}{\sqrt{2}} \left(\frac{M}{M+1}\right)^5 \ell^2 \rho\, \pi \qquad (6\text{-}46)$$

and

$$\Delta E_{\varepsilon} = -\frac{1}{3} \cdot 32 \left(\frac{M}{M+1}\right)^5 \left(\ell^2 \rho\, \pi\right)^2 \qquad (6\text{-}47)$$

For $c \neq 0$, the minimisation is not so straightforward, and it is simpler to proceed as follows. From (6-43) and (6-44)

$$\Delta E_\varepsilon = \frac{3}{4}\varepsilon^2 \omega - \frac{32\, M^3}{(1+M)^3} \cdot \frac{\ell_f^2}{c}\, \varepsilon \omega\, I(\omega) \qquad (6\text{-}48)$$

Differentiating with respect to ε gives

$$\varepsilon = \frac{2}{3} \cdot 32\, \frac{M^3}{(1+M)^3}\, \frac{\ell_f^2}{c} \cdot I(\omega) \qquad (6\text{-}49)$$

and
$$\Delta E_\varepsilon = -\frac{1}{3}\left[\frac{32\, M^3}{(1+M)^3} \cdot \frac{\ell_f^2}{c}\right]^2 \omega\, I^2(\omega) \qquad (6\text{-}50)$$

so we have the problem of finding the maximum value of $\omega\, I^2(\omega)$ or equivalently the zeros of

$$I\left(I + 2\omega \frac{dI}{d\omega}\right) \qquad (6\text{-}51)$$

Since (6-44) is a convergent integral the differentiation can be performed under the integral sign giving,

$$I + 2\omega \frac{dI}{d\omega} = \int_0^1 (1-x^2)^3 \frac{\left[(1-x^2)(1-\alpha^2x^2) - 4\omega c^{-2}(1+\alpha^2)x^2\right]}{\left[(1-x^2)(1-\alpha^2x^2) + 4\omega c^{-2}(1+\alpha^2)x^2\right]^2}\, dx$$
$$(6\text{-}52)$$

It is clearly a <u>necessary</u> condition for (6-52) to vanish that the numerator vanishes for some value of x in the range $0 < x < 1$, since all other quantities in the integrand are positive over the range of integration. However, although it is always possible to find a ω such that this condition is satisfied for any α $(-1<\alpha<1)$, (6-52) does not necessarily vanish for some finite ω. Indeed it only appears to vanish as ω tends to infinity. For the case $\alpha^2 = 1$, $(M \gg 1)$, this is easily verified, since then

$$I(\omega) = \frac{1}{2(2\omega c^{-2}-1)} \tan^{-1}(2\omega c^{-2}-1)^{1/2} \tag{6-53}$$

and $$\omega I^2(\omega) = \frac{\omega}{4(2\omega c^{-2}-1)}\left[\tan^{-1}(2\omega c^{-2}-1)^{1/2}\right]^2 \tag{6-54}$$

which increases monotonically as $\omega \to \infty$ to the limit

$$\lim_{\omega\to\infty} \omega I^2(\omega)_{\alpha^2=1} = \frac{c^2\pi^2}{32} \tag{6-55}$$

For $\alpha^2 = 0$, $(M=1)$, the integral in (6-52) may be readily evaluated and equating the result to zero gives the equation

$$\frac{1}{(t-1)^4}\left[-7t^3\,\frac{\tan^{-1}(t-1)^{1/2}}{(t-1)^{1/2}}+\left(\frac{16}{5}t^3+\frac{29}{5}t^2-\frac{38}{15}t+\frac{8}{15}\right)\right]=0 \qquad (6\text{-}56)$$

where $t = 4\omega c^{-2}$. The behaviour of the left-hand side of this equation for small t and $t \simeq 1$ is more easily seen if it is written

$$\frac{7t^3}{(t-1)^4}\left[1-\frac{(t-1)}{3}+\frac{(t-1)^2}{5}-\frac{(t-1)^3}{7}-\frac{\tan^{-1}(t-1)^{1/2}}{(t-1)^{1/2}}\right]+\frac{1}{15}\left(15t^2-6t+8\right) \qquad (6\text{-}57)$$

where $$\frac{\tan^{-1}(t-1)^{1/2}}{(t-1)^{1/2}} = \frac{\tanh^{-1}(1-t)^{1/2}}{(1-t)^{1/2}} \qquad (6\text{-}58)$$

if $t < 1$.

Equations (6-56) and (6-57) appear to have no solution other than at $t = \infty$. From this result and from the fact that as ω tends to infinity

$$\lim_{\omega \to \infty} \omega\, I^2(\omega) = \frac{c^2\pi^2}{16(1+\alpha^2)} \qquad (6\text{-}59)$$

which increases as α^2 decreases in the range $-1<\alpha<1$, we infer that the maximum value of $\omega I^2(\omega)$ for any α^2 is the result (6-59). However if we try and interpret this result in terms of the model used by Feynman to obtain his trial action, we run into difficulty. Feynman's model is that of the impurity bound harmonically to another particle of mass m. In the perturbation theory limit both the spring constant K of the binding and the mass m of the second fictional particle vanish. However the limit we have here, $\omega \to \infty$, $\varepsilon \sim \omega^{-1/2}$ implies (Schultz, 1962).

$$K \sim \omega^{3/2} \rightarrow \infty$$
$$m \sim \omega^{-1/2} \rightarrow 0 \qquad (6\text{-}60)$$

The combination of these two is such that there is a resulting finite energy correction. This energy is given by equations (6-50) and (6-59) and is

$$\Delta E_\varepsilon = -\frac{1}{3} \cdot 32 \frac{M^5}{(1+M)^5} \left(\ell^2 \rho \pi\right)^2 \qquad (6\text{-}61)$$

It is not surprising that this is the same result as (6-47), since it is independent of c. The reason for this is that when ω is large only large k in the integral in (6-43) has any importance. This is more easily seen in (6-44) where it is the region of x near zero which is dominant.

It is clear from (6-60) that we have failed to find the extension of perturbation theory that we were looking for. Feynman's trial action is

$$S_1 = -\frac{1}{2}\int\left(\frac{d\underline{x}}{dt}\right)^2 dt - \frac{1}{2}C\iint\left[X_t - X_s\right]^2 e^{-\omega|t-s|}\,dt\,ds \qquad (6\text{-}62)$$

where $C = \frac{\omega}{4}\left(v^2 - \omega^2\right)$. Perturbation theory takes $C = 0$, but if $(v-\omega) \sim \omega^{1/2}$ and tends to infinity then the second term outweighs the first. Thus the expansion (6-60) fails, as $(V-\omega)$ is not small but becomes infinite as $\omega^{1/2}$, although ε itself tends to zero as $\omega^{-1/2}$.

It is reasonable to ask how much this discrepancy depends on the treatment of the hard-core interaction and in particular on the pseudo-potential (6-22). To analyse this dependence let us consider ΔE using a well-behaved function for ω_k. The simplest to use is

$$W_k = W_0 \, e^{-\beta k^2/4} \tag{6-63}$$

For convenience, let us also take $c = 0$. Then we have for ΔE from (6-13)

$$\Delta E = \frac{3}{4v}(v-\omega)^2 - \frac{\rho W_0^2}{2\pi^2} \iint_0^\infty \exp\left[-\frac{k^2}{2}\left(\frac{\tau}{M} + \frac{F(\tau)}{v^2} + \beta\right)\right] k^2 \, dk \, d\tau \tag{6-64}$$

The integration over k can now readily be performed,

$$\Delta E = \frac{3}{4}\frac{(v-\omega)^2}{v} - \frac{\rho W_0^2}{2\pi^2}\sqrt{\frac{\pi}{2}} \int_0^\infty \frac{d\tau}{\left[\frac{\tau}{M} + \frac{\omega^2}{v^2}\tau + \frac{v^2-\omega^2}{v^3}\left(1-e^{-v\tau}\right) + \beta\right]^{3/2}} \tag{6-65}$$

Let us again look for the expected extension to perturbation theory. Writing $v = (1+\varepsilon)\omega$ and expanding in powers of ε (A is a constant),

$$\Delta E = \frac{3}{4}\omega\varepsilon^2 - A\int_0^\infty \frac{d\tau}{\left[\tau\left(\frac{1}{m}+1\right)+\beta\right]^{3/2}}\left[1 - \frac{3}{2}\cdot\frac{2\varepsilon}{\omega}\,\frac{\left(1-\omega\tau-e^{-\omega\tau}\right)}{\left(\tau\left(\frac{1}{m}+1\right)+\beta\right)} + O(\varepsilon^2)\right] \tag{6-66}$$

$$= \frac{3}{4}\omega\varepsilon^2 - A\left[\frac{2}{\beta^{1/2}}\left(\frac{M}{M+1}\right) + \varepsilon\omega^{1/2}\left(\frac{M}{M+1}\right)^{5/2}\pi^{1/2}e^{\frac{\omega\beta M}{M+1}}.\,\mathrm{erfc}\left(\frac{\omega\beta M}{M+1}\right)^{1/2}\right]$$

(6-67)

The first term in the square bracket is the energy one would obtain putting $V = \omega$ i.e. the perturbation theory energy. The other two terms is the expression (6-45), which is reobtained if we let $\beta = 0$. Minimising with respect to ε in these two terms we find

$$\Delta E = \Delta E_{V=\omega} - \frac{1}{3}A^2\pi\left(\frac{M}{M+1}\right)^5\left[e^{\frac{\omega\beta M}{M+1}}\,\mathrm{erfc}\left(\frac{\omega\beta M}{M+1}\right)^{1/2}\right]^2$$

(6-68)

and

$$\varepsilon\omega^{1/2} = \frac{2}{3}A\pi^{1/2}\left(\frac{M}{M+1}\right)^{5/2}\left[e^{\frac{\omega\beta M}{M+1}}\,\mathrm{erfc}\left(\frac{\omega\beta M}{M+1}\right)^{1/2}\right]$$

(6-69)

Putting $\beta = 0$ we again have the results (6-46) and (6-47), i.e. $\varepsilon\omega^{1/2}$ is constant and so the expansion in powers of ε is not the expected extension of perturbation theory as demonstrated above. Moreover if $\beta \neq 0$, then (6-68) is minimised when $\omega = 0$ and again $\varepsilon \omega^{1/2}$ is a constant. Thus it would appear that the expansion used by Feynman is not even valid for as well-behaved a potential as a Gaussian.

Finally it should be remarked that extending to expansion to order ε^2 does not improve matters. If we write

$$\Delta E = \frac{3}{4}\omega \varepsilon^2 - \varepsilon A(\omega) + \varepsilon^2 B(\omega) + O(\varepsilon^3) \qquad (6\text{-}70)$$

and minimise with respect to ε, we find

$$\Delta E = -\frac{1}{2} \frac{A^2(\omega)}{\left[\frac{3}{2}\omega + 2B(\omega)\right]} \qquad (6\text{-}71)$$

We have seen above that $A^2(\omega)$ behaves as ω for large ω so (6-71) has a minimum for finite ω only if $B(\omega) \sim \omega^p,\ (p > 1)$ for large ω. However when ω is large, we may replace the Bogolubov spectrum by a parabolic one i.e. let $c = 0$, since only large k is important. If $c = 0$, it is easy to see from (6-66) that if $\beta = 0$, the dependence on ω of $A(\omega)$, $B(\omega)$ and any coefficient of higher order ε is $\omega^{1/2}$. Thus for the hard-core pseudo-potential the unevaluated terms make no difference.

6. Discussion.

Although this chapter was opened in the hope that the path-integral techniques might provide some insight into the mode of behaviour of the untrapped impurity, we have to close it with the unfortunate conclusion that the method used is inapplicable to the problem. We cannot even indicate the region of applicability of perturbation theory techniques as we have been unable to obtain meaningful results when we attempt to extend them. What is not clear at present, is whether the difficulty we have found is a mathematical or a physical one. The trial action functional is sufficiently general to be capable of simulating the behaviour of the electron. Yet this very generality leads us into mathematical difficulties. Until we have found a better way of evaluating the integral in (6-13) for all ranges of the variables V and ω, we cannot improve on the perturbation theory result and test the validity of the trial action. This point is certainly worth further investigation, if only for the light it sheds on Feynman's method and on the application of path-integral techniques to Hamiltonians of the form (6-11).

CHAPTER 7.

THE NEGATIVE ION IN A FERMI SYSTEM.

1. Introduction.

In the earlier parts of this thesis, we have been exclusively working with boson systems and have shown that when there is a strong repulsive interaction between the system and an impurity, the impurity becomes self-trapped and creates a bubble around itself. Now boson systems are characterised by the existence of a ground state with long-range order and it is essentially the distortion of this state that we have considered to be the formation of the bubble. We have been able to do this because at low temperatures it is legitimate to equate the local density of the bosons with the local density of the ground state. However, having made this correlation, it is not clear how much the results depend on the boson statistics or to what extent they are 'hydrodynamic' results, i.e. that the bubble would exist in any liquid that has a sufficiently strong interaction with the impurity. The criterion on which the existence of the bubble depends is in fact independent of the statistics of the system. The criterion is that the energy of the trapped impurity must be higher than any energies associated with the surrounding medium, or equivalently, that the frequency of the motion of the impurity is rapid compared to those of the atoms containing it. Stated thus, it is clear that the statistics the atoms obey only effect the bubble insofar as they determine the energies of the individual atoms. Hence it should be possible for a self-trapped state to exist in a Fermi system as well as in a boson system, provided only that the Fermi energy is less than the energy of the trapped impurity. To demonstrate this, let us consider an imperfect Fermi gas and use the Thomas-Fermi approximation to obtain the variation in density of the fermions.

2. The Equation of Motion.

The basic equation for the energy E_1 of the impurity in this system is

$$-\frac{\hbar^2}{2\mu}\nabla^2\phi + \phi\int W(\underline{x}-\underline{x}')\,\rho(\underline{x}')\,d^3x' = E_1\phi \qquad (7\text{-}1)$$

where we assume that the impurity may be described by a wave-function $\phi(\underline{x})$ whose behaviour is governed by its interaction with the density of the fermions. With the Thomas-Fermi approximation, we have that the density is determined by the condition that the maximum energy per particle E_2 of the fermion system at any point is constant ;

$$E_2 = \frac{\hbar^2}{2M}\left(3\pi^2\rho(x)\right)^{2/3} + \int V(\underline{x}-\underline{x}')\,\rho(\underline{x}')\,d^3x' + \int W(\underline{x}-\underline{x}')\,\phi^2(\underline{x}')\,d^3x' \qquad (7\text{-}2)$$

We will again use the pseudo-potential form of the potentials discussed in Chapter 3.

$$V(\underline{x}-\underline{x}') = \frac{8\pi a\hbar^2}{2M}\,\delta(\underline{x}-\underline{x}') \qquad (3\text{-}18)$$

$$W(\underline{x}-\underline{x}') = \frac{8\pi \ell\hbar^2}{4\mu}\,\delta(\underline{x}-\underline{x}') \qquad (3\text{-}19)$$

Inserting these into (7-1) and (7-2) and letting $\hbar = \mu = 1$ we obtain the following pair of equations,

$$\nabla^2 \phi(x) + 2E_1 \phi(x) - 4\pi \ell \rho(x) \phi(x) = 0 \qquad (7\text{-}3)$$

$$(3\pi^2 \rho)^{2/3} + 8\pi a \rho(x) + 4\pi \ell M \phi^2(x) - 2E_2 = 0 \qquad (7\text{-}4)$$

The quantity E_2 can be immediately determined from the condition that $\phi(\underset{\sim}{x})$ vanishes at large distances from the origin and that $\rho(\underset{\sim}{x})$ there is the undisturbed fermion density.

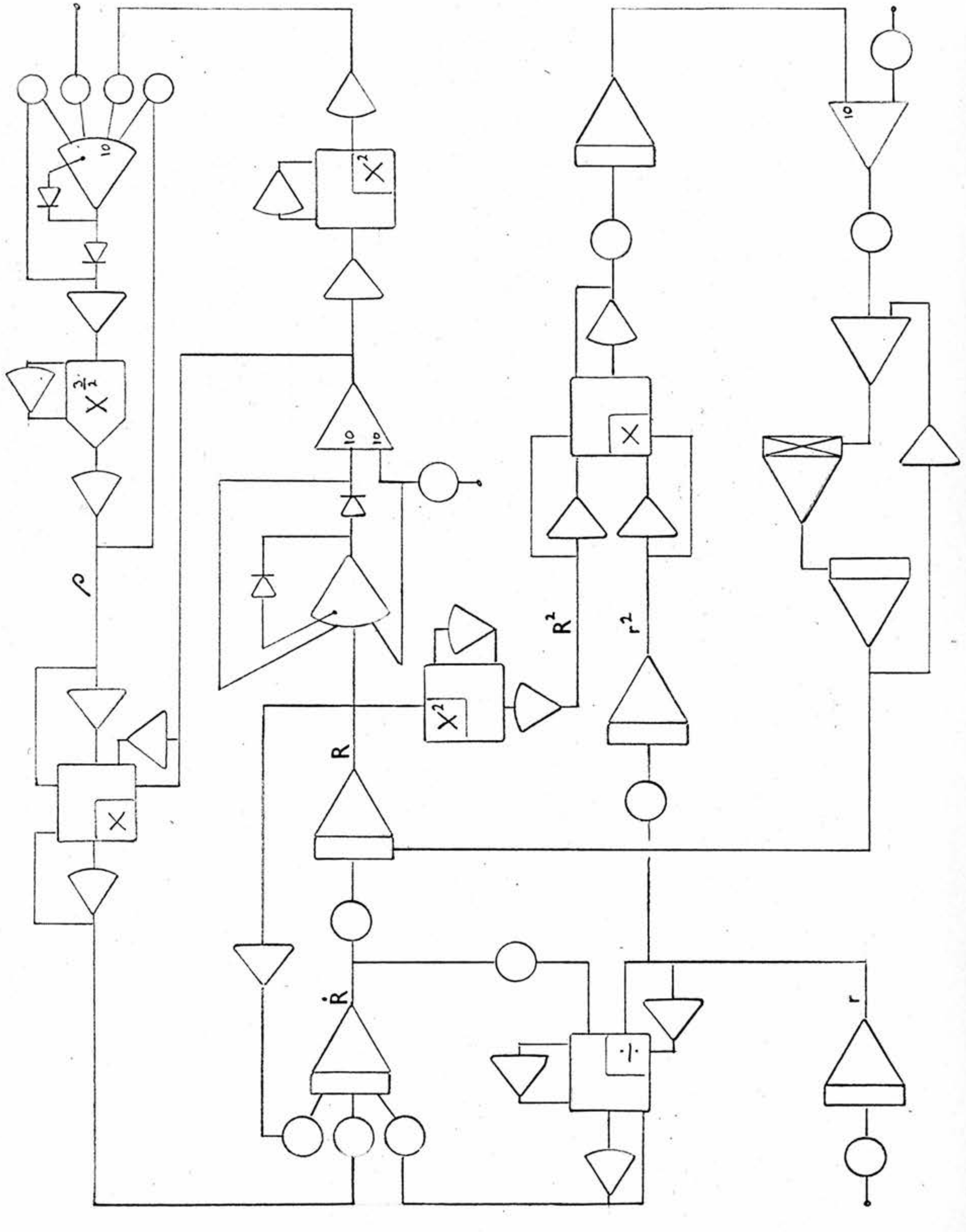
$$2E_2 = \left(3\pi^2 \rho(\infty)\right)^{2/3} + 8\pi a \rho(\infty) \qquad (7\text{-}5)$$

Moreover since $\rho(x)$ can never be negative, it is clear from (7-4) that the density vanishes everywhere that

$$2\pi \ell M \phi^2(\underset{\sim}{x}) \geqslant E_2 \qquad (7\text{-}6)$$

It is this condition together with the normalization of the function $\phi(x)$ that determines the size of the cavity in the fermion system. The

Figure 7.1.



behaviour of $\phi(\underline{x})$ is determined by (7-3) which can be reduced to a second-order non-linear equation dependent on ϕ only by substituting for $\rho(\underline{x})$ from (7-4). The resulting equation is only valid if (7-6) is violated. If (7-6) is satisfied then $\phi(\underline{x})$ satisfies,

$$\nabla^2 \phi(\underline{x}) + E_1 \phi(\underline{x}) = 0 \qquad (7\text{-}7)$$

3. Analogue Computation.

Equations (7-3) and (7-4) can be readily reduced to radial equations (neglecting angular momentum states) and in this form were set up on a PACE TR 48 analogue computer. In view of the fact that this technique has already been fully discussed in Chapter 3., we will restrict comments here to those specific to the problem.

As has been pointed out already the equations can converted into a single non-linear differential equation, so they are much simpler to handle than the pair of coupled differential equations we discussed above. Since there are only two boundary conditions to be satisfied, namely $dR/dr\big|_{r=0} = 0$

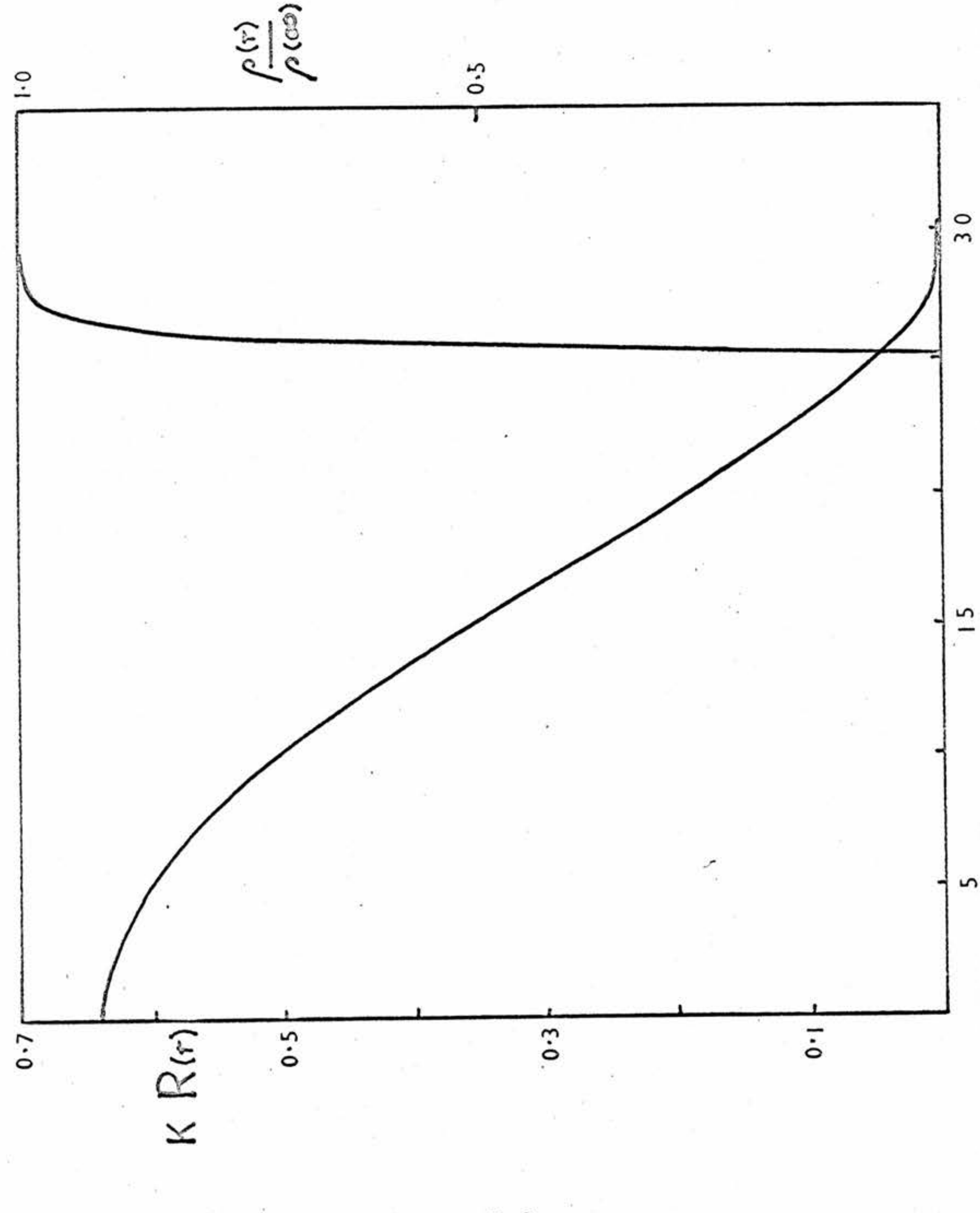


Figure 7.2.

and $\lim_{r\to\infty} R(r) = 0$ where $R(r)$ is the radial part of $\phi(\underline{r})$, the machine can be made to hunt solutions that satisfy the integral condition. One has only then to vary E_1 manually in order to find the solution that satisfies the boundary condition when r is large.

The analogue programme is shown in Figure 7.1. and the solution in Figure 7.2.. Figure 7.3. shows a sequence of solutions in a typical machine hunt for that solution which satisfied the integral condition. In this sequence, E_1 was virtually at its correct value and the final trial solution is tending to zero as r increases. If E_1 had been set too large the solution would have cut the r-axis, too small then the solution would never have reached the axis. For clarity only on the final run was the function $\rho(r)$ plotted. The negative values of $\rho(r)$ have no significance.

High accuracy was not sought in this calculation in view of the crudity of the Thomas-Fermi approximation, particularly in the vicinity of the boundary. The parameters however were selected so that easy comparisons with more realistic

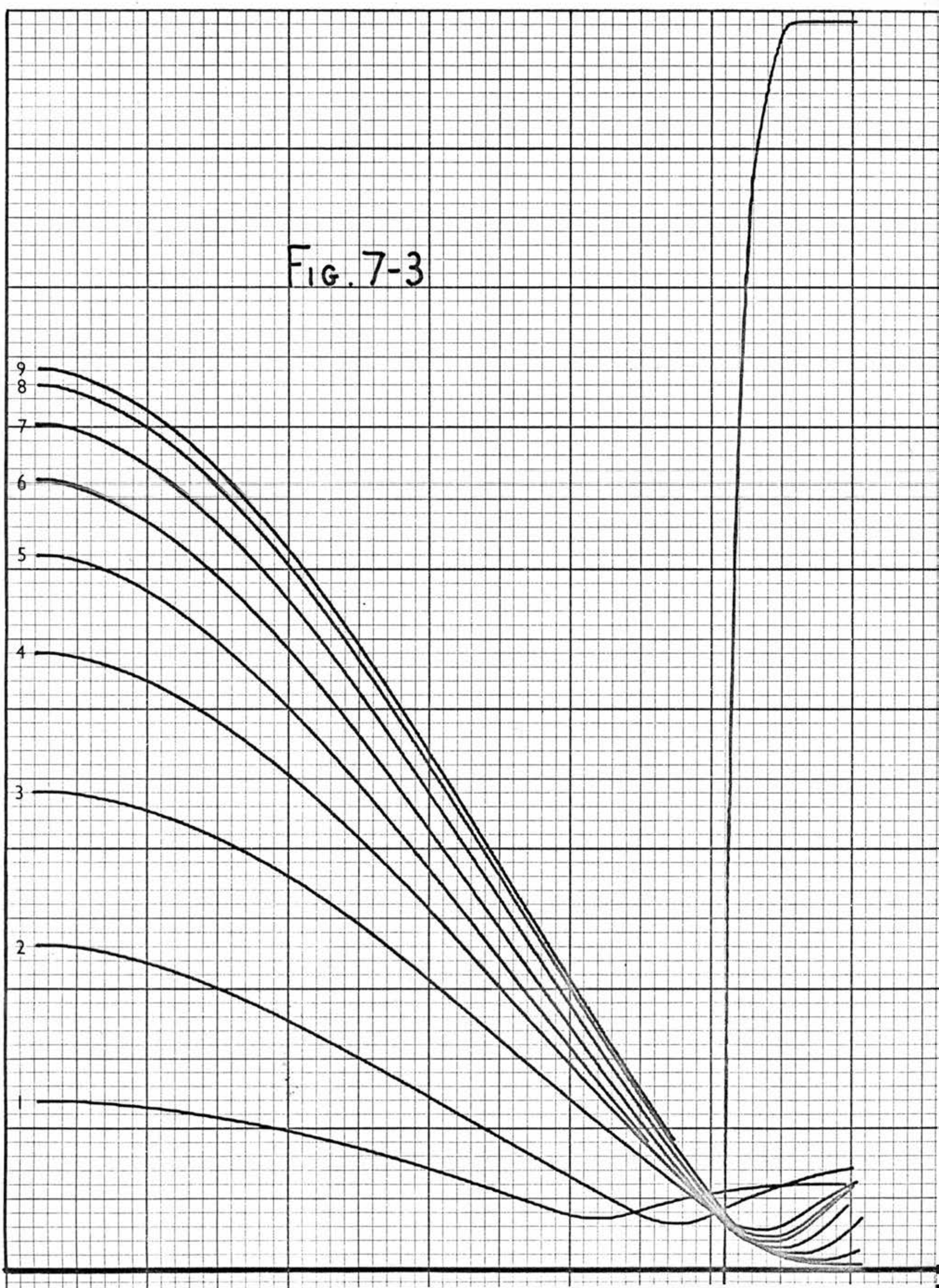


Fig. 7-3
9
8
7
6
5
4
3
2
1

predictions of the ionic cavity radius in He^3 could be made. The values used were

$$\frac{M}{\mu} = 5.47 \times 10^3 ; \quad \frac{\ell}{a} = 0.5 \quad ; \ E_2 a^2 = 5.31 \qquad (7\text{-}8)$$

The functions plotted in Figure 7.2. and Figure 7.3. are the dimensionless fermion density $\rho(r) / \rho(\infty)$ and $K R(r)$, the radial part of $\phi(\underset{\sim}{x})$ times a scale factor K chosen so that $K R$ is dimensionless,

$$K = 25 \left(\frac{2a}{3\pi}\right)^{3/2} \qquad (7\text{-}9)$$

In Figure 7.3. the vertical units are only meaningful for the function $K R$. The units along the x-axis are such that one small division is $a / 3\pi$ in length. If a is taken to be the diameter of a helium atom (2.6Å) the scale is such that the point at which $\rho(r)$ vanishes is 14.1 Å. The energy of the trapped particle is 0.08 eV, if we take its mass to be an electronic mass, which is a factor 10^2 larger than E_2, the maximum energy per particle of the fermions. Hence the criterion stated at the beginning of this chapter is satisfied.

4. Discussion.

Although the calculation cannot be applied with any confidence to liquid He^3, it is interesting to compare the computed radius with a phenomenological estimate based on Kuper's calculation (1961) in liquid He^4. It is simple to adapt his calculation. The pressure exerted outwards by the electron has to be equated to the inward pressure of the zero-point motion of the atoms minus the van der Waals pressure. There is also a small electrostriction term.

$$\frac{\pi \hbar^2}{4\mu b^5} = E_0 \rho - P_{vdW} + \rho \frac{e^2 \alpha}{2 b^4} \qquad (7\text{-}10)$$

Taking the values $E_0 = 1{\cdot}74 \times 10^{-15}$ ergs/atom (London, 1954) and $\rho = 1{\cdot}65 \times 10^{22}$ atoms/cc we find the equation

$$\begin{aligned} \frac{95{\cdot}6 \times 10^5}{b^5} &= 27{\cdot}8 - 15{\cdot}2\left(1 - \frac{(3{\cdot}9)^2}{b^2}\right) + \frac{3{\cdot}86 \times 10^4}{b^4} \\ &= 12{\cdot}6 + \frac{2{\cdot}31 \times 10^2}{b^2} + \frac{3{\cdot}86 \times 10^4}{b^4} \end{aligned} \qquad (7\text{-}11)$$

where b is expressed in Angstroms. Since the last two terms are small we can solve this equation by successive approximations. We find the solution,

$$b = 14 \cdot 57 \text{ Å} \tag{7-12}$$

which is surprisingly close to the computer solution. We feel that this is fortuitous, since the imperfect Fermi gas is not a good model of He^3 . But the fact that the two values found are close, together with the same proximity in the case of He^4 , indicates that the radius is more strongly dependent on the parameters of the liquid than on the model. It should be noted, however, that the only other published estimate of the bubble radius in He^3 (20 Å) differs wildly from the above (Clark, 1963).

CHAPTER 8.

FURTHER PROBLEMS AND CONCLUSION.

1. The Pressure Dependence of the Ions.

The bubble model of the negative ion has been successful in explaining the observed mobility of the negative ion at low fields and also provides a basis for discussion of phenomena such as the Careri steps (Careri, Cunsolo and Mazzoldi, 1961). But the mobilities of both the positive and negative ions and their step-like behaviour with increasing field are qualitatively similar. Thus it is only required that the theoretical models of the positive and negative ions have a similar macroscopic structure. Since the ratio of the theoretical radii of the ions is the same as the ratio of the experimental critical drift velocities at which the Careri steps occur, we have reasons to think that the models are correct. Apart from this indirect evidence, the ex-

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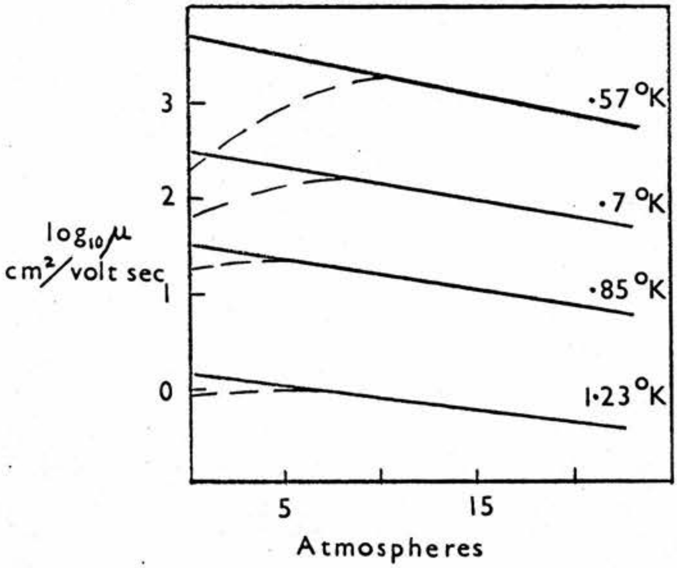

———— positive ion.

— — — negative ion.

Figure 8.1. (after Meyer and Reif, 1961).

periments do not critically differentiate between the models of the ions. Where the behaviour of the ions differs drastically is in the observed pressure dependence of the mobilities (Meyer and Reif, 1961, and Cunsolo and Mazzoldi, 1961). This is shown in Figure 8.1.. The behaviour of the mobility of the positive ion under pressure can be explained straightforwardly. The mobility is governed by collisions between the ion and rotons. The known change in number density of rotons with pressure accounts well for the observed change in the mobility. This theory also accounts for the behaviour of the mobility of the negative ion above 10 atmospheres. Below 10 atmospheres the behaviour of the negative ion mobility is strikingly different. At zero pressure the mobility is substantially lower that that of the positive ion and, as the pressure increases, the mobility increases to a value close to that of the positive ion, from which it then steadily decreases.

The difficulties associated with explaining this behaviour on the basis of the bubble model are manifold. If one accpets Atkins (1959) electrostriction model of the positive ion, one can explain the above mobility change by postulating that the model is virtually pressure independent. This can be forced on the theory by assuming that the growth of the central solid core (if it exists), as the external pressure approaches the melting pressure, is restricted by surface tension (Atkins, 1959, 1963). Above 10 atmospheres we must assume that electrostriction effects play a dominant role in determining the mobility of the negative ion as well. This implies that radius of the bubble decreases steadily from about 12 Å at zero pressure to a value approximately that of the radius of the positive ions core (6 or 7 Å) as the pressure increases. However this requires that the bubble model is very much more sensitive to pressure than Kuper's (1961) calculation allows. If this calculation is taken as a basis, a change of 10 atmospheres in the external pressure would reduce the radius of the bubble by less than one Angstrom, i.e. less than 10%, whereas a change of the order of 50% is needed.

The only concept that could explain such a behaviour is that of electron penetration into the liquid. Kuper assumes that the electron is virtually in an infinite potential well and we have seen in earlier chapters that this is not a bad approximation. As the pressure increases however, the penetration will become larger and the electrostrictive forces will play a more important part in determining the radius of the bubble. This may cause the bubble radius to be strongly pressure dependent. This theory certainly merits further investigation.

The rough idea of the collapsing bubble was mentioned in a footnote by Kuper (1961) and was also conceived by Cunsolo and Mazzoldi (1961). Neither of these authors have worked out any details.

2. The Transition from the Free to the Trapped Mode.

A second problem of some interest is an adequate treatment of the transition of the electron from the self-trapped state to the conduction band behaviour. As we have seen in Chapter 6., path-integral techniques seem to be inapplicable beyond the perturbation theory limit. In any case, we would not expect the theory to apply to the bubble mode because of the assumption in developing the Hamiltonian of the validity of the expansion into plane wave states. At present, the best that can be done, in order to predict the density at which the transition occurs, is to compare the energy given by perturbation theory with the energy of the bubble structure at various densities and choose that density at which they are equal to be the transition density. This has been done (in a paper to be published) by Jortner, Kestner, Rice and Cohen. Their perturbation theory differs from ours in that it assumes that the helium atoms occupy rigid sites, whereas the polaronic perturbation theory allows the atoms to recoil. Their estimate of the bubble radius (21 Å) also differs from ours as they assume that the radius is determined by the external pressure not by the zero-point pressure of the atoms as we have done. Their calculation however is aimed at determining the structure of the negative ion in helium gas as it is only in densities as low as those of the gas that one obtains the transition. The density at which they find the transition should occur is $0{\cdot}9 \times 10^{21}$ atoms/cc , which in terms of the coupling constant defined in Chapters 3. and 4. is $\alpha = 1{\cdot}11 \times 10^{3}$. This is a factor 5 larger than the minimum α found in Chapter 4. but as remarked there, the model could not describe the free-electron so could not be expected to give more than an order of magnitude.

This argument is quite crude but the result is in fair agreement with the density at which a sharp drop in the negative ions mobility occurs (Levine and Sanders, 1962). The experimental values of the mobility drop rapidly over four orders of magnitude as the density is increased between the values $0{\cdot}6 \times 10^{21}$ atoms/cc and $1{\cdot}5 \times 10^{21}$ atoms/cc. There seems little doubt that this drop is caused by the transition from the free electron state to the trapped state, particularly in view of the agreement with theory, but the mechanism is not altogether clear as the pressure required for the mobility drop to occur is close to the saturated vapour pressure and hence the pure gas model may not be valid. Apart from this one reservation, we believe that the result is additional evidence in support of the bubble theory. It is fair to say, however, that the theories that describe the motion of the electron above and below the transition fail in the region of the transition. A theory that covers both limits and the transition region remains unknwn.

3. Conclusion.

In this thesis we have attempted to put the bubble model of the negative ion on a firm theoretical basis and to calculate from first principles some of its characteristics. Whether we have succeeded depends on the judgement of the reader. There remain many problems most of which we hope we have outlined in the body of this work. The behaviour under pressure, the effect of polarization, the transition to the free state, the effect of collisions with excitations in the helium, further excited states of the ion, in particular rotational states and deformed configurations are but a few of these problems. What is certain is that there now exists a body of work on the structure of the negative ion, to which we have contributed a little and from which discussion of these further problems can proceed.

APPENDIX A.

THE EQUATION $R'' + \frac{2}{r}R' + R - R^3 = 0$.

In this appendix, the non-linear, non-autonomous second-order differential equation

$$R'' + \frac{2}{r} R' + R - R^3 = 0 \qquad \text{(A-1)}$$

will be studied. Primes denote differentiation with respect to r. Equation (A-1) has three trivial solutions,

$$R = 0 , 1 , -1 \qquad \text{(A-2)}$$

The solutions $R = \pm 1$ divide all solutions that obey the boundary condition, $R' = 0$ at $r = 0$, into three distinct types ; (a) $|R(0)| < 1$, (b) $R(0) > 1$, (c) $R(0) < -1$. Type (a) perform damped oscillations about $R = 0$, types (b) and (c) diverge monotonically to $+\infty$ and $-\infty$ respectively.

More specifically the following theorems can be proved.

<u>Theorem 1.</u> (a)

If $X(r)$ is a solution of (A-1), continuous and with continuous derivatives, and $X'(r) = 0$ for some value of r, $r = k$ say, such that $X(k) > 1$, then $X(r) > 1$ for all $r > 0$ and $X'(r) > 0$ for all $r > k$, and $X'(r) < 0$ for all $0 < r < k$.

Proof : If $X'(k) = 0$ then from (A-1)

$$X''(k) = X^3(k) - X(k) > 0 \qquad (A-3)$$

Hence $X(k)$ is a minimum of $X(r)$ in the (X, r) plane. Hence for some $\delta > 0$, $X'(k+\delta) > 0$ and $X'(k-\delta) < 0$, and $X(k \pm \delta) > X(k)$. Hence $X'(r) > 0$ for all $r > k$ and $X'(r) < 0$ for all $0 < r < k$. Since if $X'(r) = 0$ for some $r > k$, let $r = \ell$ be the first value of r at which $X'(\ell) = 0$. Then $X(\ell)$ must be a minimum. Hence, since $X'(r)$ is continuous and $X'(k+\delta) > 0$ and $X'(\ell - \delta) < 0$, there exists some r in $k + \delta < r < \ell - \delta$ at which $X'(r) = 0$, which contradicts the assumption that ℓ was the first value of $r > k$ at which $X'(r)$ vanished. Similarly for $r < k$.

Q.E.D.

Similar theorems can be proved for the cases

(b) $X(k) < -1$

(c) $0 < X(k) < 1$ (A-4)

(d) $0 > X(k) > -1$

In case (b) $X(k)$ can be proved to be a maximum and $X'(r) > 0$ for all $0 < r < k$ and $X'(r) < 0$ for all $r > k$. In (c), $X(k)$ is also a maximum and $X'(r)$ cannot change sign at any $r = \ell \neq k$ unless $X(r)$ vanishes in the open interval (ℓ, k). In (d), $X(k)$ is a minimum and $X'(r)$ similarly cannot change sign at $r = \ell$ unless $X(r)$ vanishes in (ℓ, k). Theorems (b) and (d) can be deduced from (a) and (c) by observing that (A-1) is unaltered under the transformation $R(r) \to -R(r)$, i.e. reflexion in the $r = 0$ axis in the (R, r) plane.

The substitution $R = \frac{1}{r}\chi(r)$ reduces (A-1) to

$$\chi'' + \chi - \frac{\chi^3}{r^2} = 0 \qquad \text{(A-5)}$$

If the maximum value of $\chi \ll r$, the solutions of (A-5) tend asymptotically to the solutions of

$$\chi'' + \chi = 0 \qquad \text{(A-6)}$$

However, in Chapter 3., we are more interested in solutions that behave asymptotically as $R = 1$, so for large r, write,

$$\chi = r + \delta(r) \qquad \text{(A-7)}$$

where $\delta(r)$ is small, and $\to 0$ as $r \to \infty$. Then

$$\chi'' + \chi - \frac{\chi^3}{r^2} = \delta'' + (r+\delta) - \frac{(r+\delta)^3}{r^2} = 0 \quad \text{(A-8)}$$

or since $\delta(r)$ is small, neglecting higher order terms than the first

$$\delta'' - 2\delta = 0 \quad \text{(A-9)}$$

The solution $\delta(r) = a e^{-2r}$ satisfies the condition that $\delta(r) \to 0$ as $r \to \infty$. Hence there exists solutions of (A-1), that for large r behave as

$$Y(r) = 1 + a\frac{e^{-2r}}{r} \quad \text{(A-10)}$$

These solutions are not necessarily finite at $r = 0$, but we are interested in Chapter 3. in solutions like (A-10) that vanish for some finite $r > 0$. If in $Y(r)$, $a < 0$, from Theorem 1. (c), since for some finite $r = m$, $Y(m) < 1$ and $Y'(m) > 0$, then either for some $0 < r < m$, $Y(r)$ must vanish, or $Y(r)$ is monotonically increasing from some value $Y(0)$ at $r = 0$, $0 < Y(0) < 1$, and $Y'(0) > 0$. Now these last two conditions are mutually incompatible for the condition that $Y(0)$ is finite, implies $Y'(0) = 0$. The proof of this statement is as follows (Chandrasekhar, 1939, proves this theorem for the equation $R'' + \frac{2}{r} R' + R^n = 0$. We merely adapt his proof here).

The solutions of (A-1) that are finite at the origin in the (R, r) plane correspond to solutions of (A-5) that pass through the origin in the (χ, r) plane. Also

$$\frac{dR}{dr} = \frac{1}{r}\frac{d\chi}{dr} - \frac{\chi}{r^2} \qquad \text{(A-11)}$$

Hence
$$\left(\frac{dR}{dr}\right)_{r=0} = \lim_{r \to 0}\left(\frac{1}{r}\frac{d\chi}{dr} - \frac{\chi}{r^2}\right) \qquad \text{(A-12)}$$

Expanding $\chi(r)$ and $\chi'(r)$ in a Taylor series about $r = 0$

$$\chi(r) = 0 + r\,\chi'(0) + \frac{r^2}{2}\chi''(0) + \cdots$$

and
$$\chi'(r) = \chi'(0) + r\,\chi''(0) + \cdots$$

and substituting in (A-12) gives

$$\begin{aligned}\left(\frac{dR}{dr}\right)_{r=0} &= \lim_{r \to 0}\left[\frac{1}{2}\chi''(0)\right] \\ &= \lim_{r \to 0}\left[\frac{\chi}{2}\left(\frac{\chi^2}{r^2} - 1\right)\right] \\ &= 0\end{aligned}$$

since $R = \frac{\chi}{r}$ is finite at $r = 0$, and $\chi = 0$ at $r = 0$. Hence $Y(r)$ must vanish for some finite r , since $Y'(0)$ cannot be greater than zero at $r = 0$ for

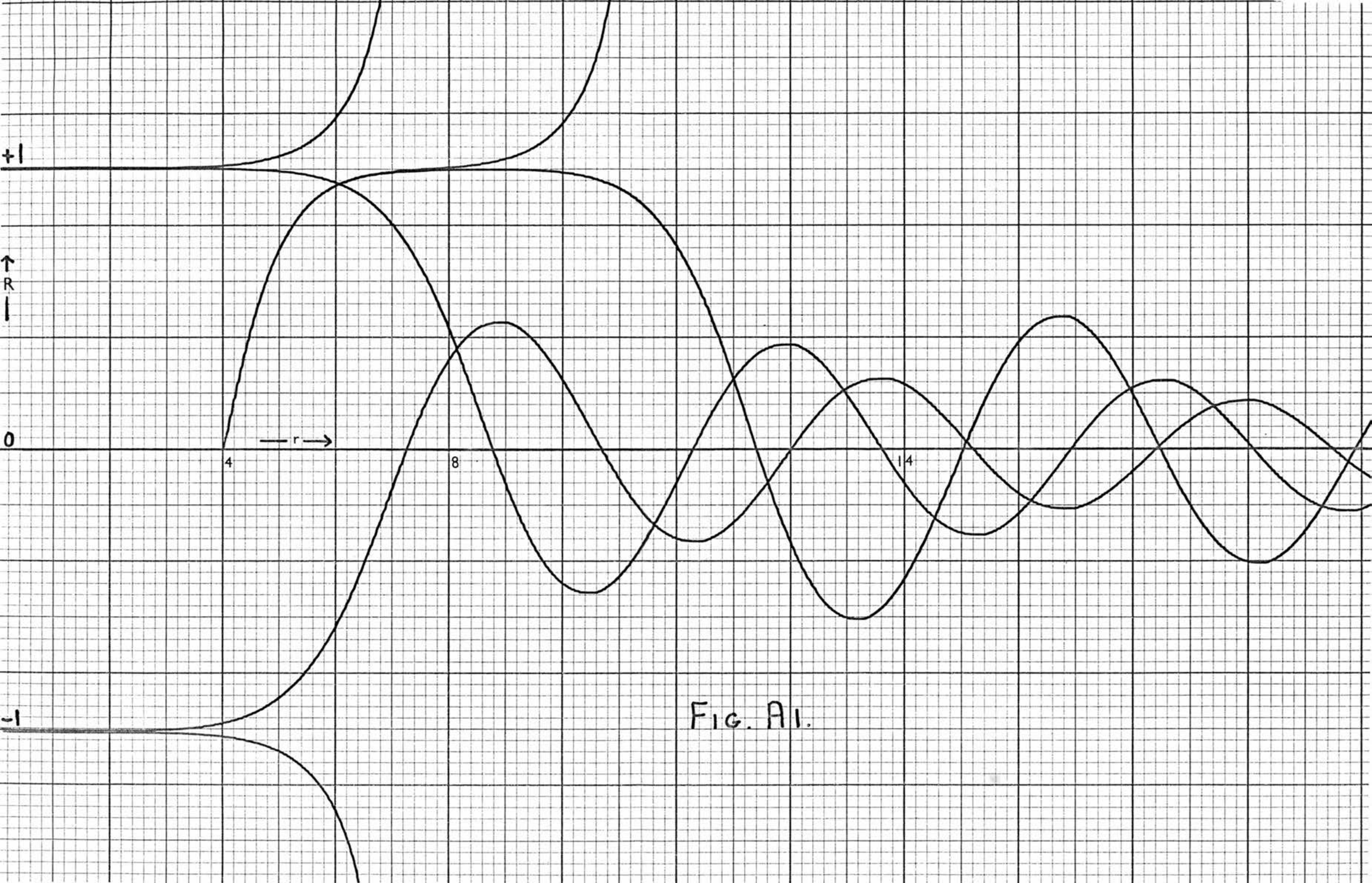

FIG. A1.

finite Y . Figure A.1. shows solutions that have $R' = 0$ at $r = 0$ and $R(0) \approx 1$. Also shown in Figure A.1. are two solutions that vanish at $r = 4$ and are upper and lower bounds to the solution that satisfies the condition that $R \to 1$ as $r \to \infty$. The solution that satisfies this condition lies between these two.

The two solutions $R = 1$ and $R = -1$ are unstable. This is easily seen from Figure A.2. which shows the phase-plane diagram of solutions of (A-1) which are finite at the origin. The solutions $R = 1$, $R = -1$ are the points $(0, 1)$ and $(0, -1)$. Unstable solutions are characterised by saddle-points in a phase-plane diagram. Stable points, such as $(0, 0)$, are characterised by lines that spiral into them. To find the separatrices, we observe that they result from the limiting solutions above and below $R = 1$ or $R = -1$. Hence, since we can always find a solution such that given r , $\left(\frac{1}{r}\frac{dR}{dr}\right)$ is negligible at r , the separatrices result from the limiting solutions of

$$R'' + R - R^3 = 0 \qquad \text{(A-13)}$$

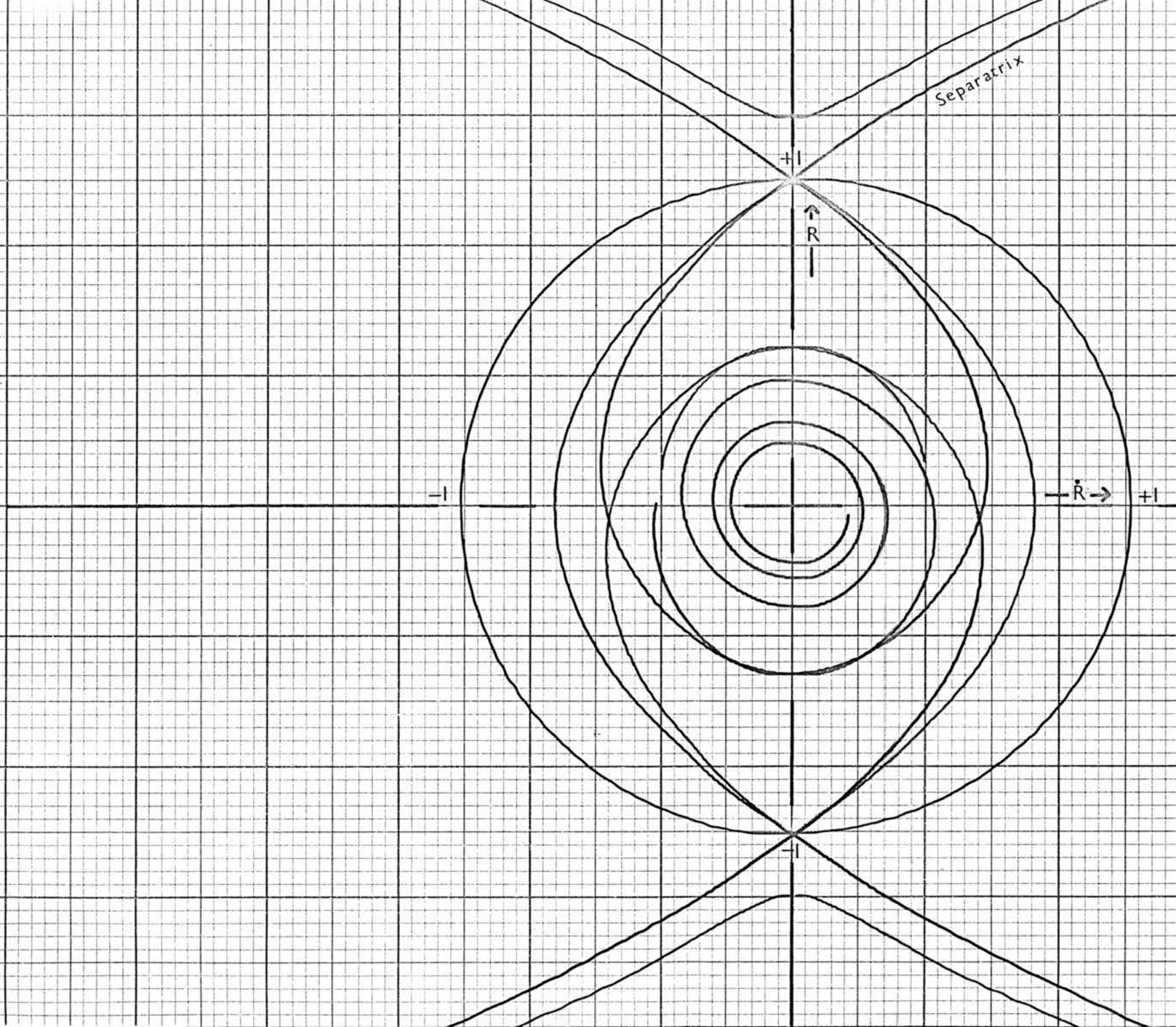

FIG. A2.

for which $R'(0) = 0$, and $R(0) = 1+\delta$, as $\delta \to 0$. Let $y = R(r)$ and $x = R'(r)$, where $x = 0$, $y = 0$ are the coordinate axes in the phase-plane. Then

$$R'' = \frac{dx}{dr} = R^3 - R = y^3 - y \qquad \text{(A-14)}$$

and $$\frac{dy}{dr} = R' = x \qquad \text{(A-15)}$$

Hence the separatrices are given by the solutions of

$$\frac{dx}{dy} = \frac{y^3 - y}{x} \qquad \text{(A-16)}$$

which pass through the points $(0,1)$, $(0,-1)$. These are the two parabolae

$$y^2 = \left(1 \pm \sqrt{2}\, x\right) \qquad \text{(A-17)}$$

enclosing the origin.

The separatrices are drawn in Figure A.2.. Also for comparison, is shown the phase-plane diagram of the solutions of

$$R'' + R = 0 \qquad \text{(A-18)}$$

that satisfy $R' = 0$, $R = 1$ at $r = 0$.
Equation (A-13) is, of course, a special case of the equation whose solutions are Jacobean ellip-

tic functions. The solutions of more general equations, $\left(1 \geq m \geq 0 \ , \ a \text{ real} \right)$,

$$R'' + \frac{a^2}{2}(1+m)R - a^2 R^3 = 0 \qquad \text{(A-19)}$$

$$R'' + \frac{a^2}{2}(1+m)R - a^2 m R^3 = 0 \qquad \text{(A-20)}$$

that satisfy the boundary conditions $R'(0) = 0$, $R(0) = 1$, are $dc\left(\frac{ar}{\sqrt{2}} \middle| m\right)$ and $cd\left(\frac{ar}{\sqrt{2}} \middle| m\right)$ respectively. As $m \to 1$, $a \to 1$ both these solutions degenerate to the line, $R(r) = 1$.

Finally we list a few alternative forms of (A-1) that might be useful for special purposes.

i) $R = \frac{1}{r}\chi(r) \quad ; \quad \chi'' + \chi - \frac{\chi^3}{r^2} = 0$

ii) $R = \frac{\cos r}{r}\chi(r) \quad ; \quad \chi'' + 2\tan r . \chi' - \frac{\cos^2 r}{r^2} . \chi^3 = 0$

iii) $R = \chi(t), \ r = \frac{a}{t+b} \ ; \quad \frac{(t+b)^4}{a^2}\ddot{\chi} + \chi - \chi^3 = 0$

iv) $R = e^t \chi(t), \ r = e^{-t} ; \quad \ddot{\chi} + \dot{\chi} - \chi^3 + e^{-2t}\chi = 0$

where $\dot{\chi} = \frac{d\chi}{dt}$

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