A Fermi-Thomas Type Method for Atoms and Nuclei

Thesis submitted for the Degree of

Doctor of Philosophy

in

The Australian National University

by

Mihir Kumar Roy
ACKNOWLEDGEMENT

My thanks are due to my supervisors Prof. K.J. Le Couteur and Dr. K. Kumar who suggested this work, and helped and guided me throughout its progress. My indebtedness to them cannot be overestimated.
The work reported in this thesis is the result of the research done by me during the period March 1961 to February 1964, when I was a research scholar in the Australian National University. Parts of it have been published in Scientific Journals under the joint authorship of Prof. K.J. Le Couteur, Dr. K.Kumar and myself. The parts which are done by me and the parts which are done jointly with Prof. Le Couteur and Dr. Kumar are indicated below.

Chapter I : This contains reviews done by me of some standard works by other people.

" II : With a brief introduction this chapter goes on to report some new work done by me jointly with Prof. Le Couteur.

" III : The work reported in this section was done separately by Dr. Kumar and myself (Section 1).

Section 2. The work here was done by me jointly with Dr. Kumar.

Section 3. The work reported here was done by me.

Section 4. This was done by me.

Section 5. It is a joint piece of work done by me with Prof. Le Couteur and Dr. Kumar.
Chapter IV : Section 1. Dr. Kumar was responsible for the work done in this section.

Section 2. (i) & (ii) were done by me jointly with Prof. Le Couteur and Dr. Kumar.

\[ V \quad : \quad \text{Sections 1 & 2. Each of us three (Prof. Le Couteur, Dr. Kumar and myself) worked together and separately.} \]

Appendix : The numerical method is due to Prof. Le Couteur.

M. K. Roy
22. 2. 65
In the presentation of this thesis we have followed the following conventions. Chapters are denoted by Roman numerals I, II etc. Sections are denoted by ordinary numerals 1, 2 etc. Sub-sections are denoted by i, ii etc. The equations in each section have the section number followed by the equation number, i.e. eq. (2.3) means the 3rd equation in the 2nd section of a particular chapter. No separate numbering for the sub-sections are done, i.e., all the equations in a section have the section number irrespective of the sub-sections. When references are made for an equation in the same chapter we use only the section number along with the equation number, i.e., if in the third chapter we refer to eq. (2.3) it will mean the 3rd equation in section 2 of the third chapter. If we want to refer to an equation in another chapter, we write the chapter number followed by the section and equation numbers, e.g., if in the 5th chapter we refer to the 3rd equation of section of chapter III, we write it as eq. (III. 2.3).
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References
The Quantum Mechanics of even a three-body system is not properly understood. So it would seem rather difficult to imagine that the quantum mechanics of many-body systems could be solved easily. Fortunately there is a good approximation to which the problem of many-body systems can be reduced. This approximation, in which the particles move as independent particles in a potential determined by averaging over all possible positions of all other particles, is called the independent particle model. In case of an atom this potential is due to all the other electrons and also to the nucleus, while in case of a nucleus it is due to all the other nucleons.

1. Hartree-Fock method for atoms

To write down Hartree-Fock equations, we start with a determinantal wave function given in terms of normalized single particle wave function as

\[
\begin{vmatrix}
\psi_1(1) & \psi_1(2) & \cdots & \psi_1(N) \\
\psi_2(1) & \psi_2(2) & \cdots & \psi_2(N) \\
\vdots & \vdots & \ddots & \vdots \\
\psi_N(1) & \psi_N(2) & \cdots & \psi_N(N)
\end{vmatrix}
\]
where \( N \) is the total number of electrons in the atom. Expression (1.1) is antisymmetric in character and automatically satisfies Pauli’s exclusion principle. \( (N!)^{-1/2} \) is the normalising factor. Each of the one-electron wave functions is assumed to be the product of a function of coordinates and a function of spin; that is, each one-electron wave function corresponds to a definite value of \( m_s \). All the spatial wave functions corresponding to a certain value of \( m_s \) will be orthogonal to each other. Then the average value of the Hamiltonian

\[
\frac{\hbar^2}{2M} \sum_{i} \frac{\mathbf{r}_i^2}{r_i} - \frac{Z}{r_i} + \sum_{i<j} \frac{e^2}{r_{ij}}
\]

will be given by

\[
(H)_{uv} = \sum_{i} \int \psi_i^*(1) \psi_i(1) d\mathbf{r}_1 + \sum_{i<j} \int \psi_i^*(1) \psi_j^*(2) \psi_j(2) d\mathbf{r}_1 d\mathbf{r}_2
\]

(1.2)

where \( \psi_i(1) \) and \( \psi_j(2) \) are the single particle wave functions at positions \( \mathbf{r}_1 \) and \( \mathbf{r}_2 \) respectively. The one-electron operator \( f_1 \) and the two-electron operator \( g_{12} \) are given in atomic units with \( \hbar = M = 1 \), as

\[
f_1 = -\nabla_1^2 - \frac{2Z}{\mathbf{r}_1}; \quad g_{12} = \frac{2}{r_{12}}
\]

(1.3)

where \( Z \) is the atomic number and the integration over \( d\mathbf{r}_1 \) and \( d\mathbf{r}_2 \) is only over the spatial coordinates.
is the Kronecker delta. $f_1$ gives the sum of the kinetic energy and the Coulomb potential energy due to the nucleus, while $g_{12}$ gives the Coulomb potential energy between two electrons. To derive the Hartree-Fock equations we want to minimise the average energy. We do this by varying the $\psi_i$'s in equation (1.2) with the subsidiary conditions of normalisation of all $\psi_i$'s and orthogonality of any two $\psi_i$'s associated with the same $m_3$. By using the method of undetermined multipliers, after a little algebraic manipulation, we get

$$\frac{1}{2} \left[ \frac{1}{\rho} \psi_c(l) + \sum_j \int \psi^*_{j}(z) g_{12} \left[ \psi_{c}(l) \psi_{j}(z) - \delta(m_{s_i} m_{s_j}) \psi_{c}(z) \psi_{j}(l) \right] d\nu_z \right]$$

$$= - \sum_j \delta(m_{s_i} m_{s_j}) \lambda_{ij} \psi_j(l)$$

(1.4)

Here we have put

$$\lambda_{ji} = \lambda_{ij}^*.$$

In order to put the Hartree-Fock equations (1.4) into a more convenient form we make a unitary transformation of the $\psi_i$'s. Such a transformation leaves the determinantal function unchanged, for it follows from the theory of determinants that a determinant whose rows or columns are found from those of another determinant by a unitary transformation is identical to the original determinant, aside from a constant factor whose absolute value is unity. Since our derivation minimises the energy, which depends only on the determinantal function as a whole, it obviously cannot choose between different forms of one-electron wave functions which lead
to identical determinants.

To investigate the effect of such a unitary transformation let us transform the \( \psi_i \)'s into a new set of \( N \) orthonormal functions, the \( \phi_j \)'s, according to a transformation equation

\[
\phi_j = \sum_k c_{kj}^* \psi_k, \quad \psi_j = \sum_k c_{jk} \phi_k
\]  

(1.5)

where, of course, \( (C_{nk})^{-1} = C_{kn}^* \).

We use a special sort of transformation. In order to preserve the form of wave functions which we are assuming, our transformation can mix \( \psi_i \)'s of the same value of \( m_s \) with each other, but not with those of the opposite \( m_s \). In other words, the coefficients \( C_{kj} \) must be zero unless the indices \( k \) and \( j \) refer to wave function with the same spin. This is equivalent to saying that the transformation can be considered as a successive application of two transformations, one of the wave function with + spin, the other of the wave functions with - spin. After some calculation we find

\[
\frac{1}{2} \phi_i (1) + \sum_j \left[ \psi_j^* (2) \phi_j (2) - \delta (m_{s_1} m_{s_j}) \phi_i (2) \phi_j (1) \right] d\nu_2
\]

\[
= - \sum_j \delta (m_{s_1} m_{s_j}) \phi_j (1)
\]  

(1.6)
We notice that when the $\psi_i$'s undergo a unitary transformation the form of the H.F. equation is not altered, but the quantities $\lambda_{ij}$ transform like the components of a matrix. Since we have put $\lambda_{ij} = \lambda_{ji}^*$, this matrix is Hermitian.

So we can conclude that a unitary transformation of the $\psi_i$'s can be found which will diagonalise the matrix $\lambda_{ij}$, so that the components $\lambda_{ij}$ form a diagonal matrix. The process of diagonalising this matrix is just like the ordinary one of solving Schrödinger's equation. The particular choice of $\phi_i$'s which gives us a diagonal matrix has specially simple properties, and we shall assume that we are dealing with solutions of the H.F. equations which have this property of diagonalising the $\lambda$ matrix.

Then, we can write the H.F. equations in the form

$$\frac{1}{2} J_{ij} \psi_i (1) + \sum_j \lambda_{ij} \psi_j (2) \frac{d}{dx} \left[ \psi_i (1) \psi_j (2) - \delta (m_{s_i} m_{s_j}) \psi_i (2) \psi_j (1) \right] du_2 = \epsilon_i \psi_i (1)$$  \hspace{1cm} (1.8)

or, using equations (1.3), we have from (1.8)

$$-\frac{L^2}{2} \psi_i (1) - \frac{2}{n} \psi_i (1) + \frac{1}{2} \left[ \sum_j \psi_j^* \left( \frac{2}{n} \gamma \right) \psi_j \right] du_2 \psi_i (1)$$  \hspace{1cm} (1.9)
where we have used $\varepsilon_i$ in place of $-\lambda_{ii}$.

$-\varepsilon_i$ represents the energy required to remove the $i$th electron from the atom. In equations (1.9) the first term represents the kinetic energy, the 2nd term the potential energy due to the nucleus, the third term the potential energy due to all the electrons of both spins and the last term the exchange potential energy.

The independent particle model is good enough for electrons in an atom. But there was no a priori reason to believe that such a model should work at all for nucleons in a nucleus. In contradistinction to the forces operating between electrons, forces between two nucleons are of short range, of great strength and probably have repulsive cores. It was very difficult to see how such forces could lead to an average potential field with a collection of non-interacting or weakly interacting nucleons moving in it, as is done in the "Shell model" of Mayer and others. In spite of this deficiency in the first step, the shell model has very good successes in explaining many properties of bound states of nuclei and of nuclear reactions. But if shell model is accepted then we have to admit that the nucleons inside a many-body medium behave to some extent like an assembly of non-interacting or weakly interacting particles and that the two-body forces are weak and long ranged and as such there is an absence of correlations in the ground-state wave.
functions. Many attempts have been made so far to explain this paradox, viz. on one side very short-ranged strong forces with complicated exchange characters and on the other side a behaviour of a nucleon inside a nucleus which looks like the behaviour in a smooth potential without large magnitude and large variation. Some people argued that the origin of this effect might be, for example, a strongly non-linear behaviour of the meson field so that a very large damping effect modifies and smooths out the forces in nuclear matter. These effects can arise for many-body forces or from a non-linearity in the meson field equation. In either case the effective potential felt by one nucleon would not have the rapidly varying spatial dependences which would result if the two-body forces remained strong even inside the nucleus and a uniform potential would be a good approximation. But there are strong arguments to show that the two-body forces continue to exist inside a nucleus and are not replaced by a general smooth potential. These arguments are summarised in a paper by Brueckner, Eden and Francis. The point is that there is abundant evidence that the nuclear wave function contains very strong components of high momentum which manifest themselves in such processes as the capture of $\pi^-$-mesons and the photoelectric effect caused by high energy $\gamma$-rays. In both cases, a large amount of energy
without much momentum is given to the nucleus. In order for a nucleon to absorb this energy, and at the same time to conserve momentum, the nucleons must have had a large momentum before it absorbed the $\Lambda$-meson or the $\gamma$-ray; i.e. the wave function of the nucleus in its normal state must contain components corresponding to large momenta of an individual nucleon. Examples like deuteron pick-up processes also give the same indication.

All these experiments show very definitely that the potential inside a nucleus is a highly fluctuating function of position, which is compatible with the idea that the two-body forces do not die down even when the pair of nucleons is immersed in a many-body medium.

There are similar difficulties in understanding the successes of "cloudy crystal ball model" and "collective model" of A.Bohr and others. They could, no doubt, explain successfully many properties of nuclei of diverse nature, but most of them only by essentially assuming the validity of some type of independent particle model.

So, when we develop a theory of nucleus at this stage, we must require that on one hand it gives us one particle features for all low energy phenomena and on the other hand it must preserve in the nuclear wave functions very strong components of high momenta. Such components can easily be
provided if we believe that the nuclear forces continue to exist inside the nucleus as they do outside the nucleus.

So the task is to use the strong two-body forces as evidenced in the free nucleon scattering experiments and to construct with these a theory of complex nuclei which can reproduce, with as good an approximation as possible, the one particle picture of the shell model. This is exactly the programme which was carried out by Brueckner and his collaborators.

2. Time dependent perturbation theory and Feynman graph analysis

We follow Goldstone's method and start with the one-particle Schrödinger equation

\[(T_i + V_i) \psi_n(i) = E_n \psi_n(i)\]  \hspace{1cm} (2.1)

whose solutions are given by the one-particle eigenstates \[\psi_n(i)\] with eigenvalues \[E_n\]. \[T_i\] and \[V_i\] are the kinetic energy and potential energy operators. This potential energy \[V_i\] may be regarded as that gained by the \(i\) th nucleon due to its encounters with all other nucleons inside the nucleus, with each of which it interacts by the interaction potential \(V_{ij}\). The exact functional dependence of \(V_i\) on \(V_{ij}\) will be explored later on. \(V_i\) will have a dependence on both spatial and momentum coordinates. The Schrödinger equation is now written in the form
Solutions of equations (2.1) or (2.2) for a potential well of finite radius will give discrete states for $E_n < 0$ and continuum states for $E_n > 0$. A state of the nucleus is defined by specifying which of the one-nucleon states $\psi_n$'s are occupied by the nucleons, and the set of occupied one-nucleon states will be called configuration. Each configuration will be described by a Slater determinant which contains only the occupied one-nucleon states. This determinant, we call, the "model wave function" and denote it by $\Phi$. $\Phi$ is an eigenstate of the "model Hamiltonian" $H_0$ which may be written as

$$H_0 = \sum_{i=1}^{A} (T_i + V_i) \quad (2.3)$$

The $A$-particle Hamiltonian $H$ of the actual problem is given by

$$H = \sum_{i=1}^{A} T_i + \sum_{i>j} V_{ij} \quad (2.4)$$

We define

$$H_1 = \sum_{i>j} V_{ij} - \sum_{i} V_i \quad (2.5)$$

so that

$$H = H_0 + H_1 \quad (2.6)$$
All expansions are made in powers of $H$. The one-nucleon wave functions $\psi_n$, represented by $|n\rangle$, are calculated from the one-particle single-particle Schrödinger equation (dropping the particle symbol $i$ or $j$)

$$(T + V)|n\rangle = E_n|n\rangle \tag{2.7}$$

The matrix elements of $V_{ij} = V$ and $V_i = V$ are defined by the relation

$$\langle rs |V| mn\rangle = \int \psi_r^*(i) \psi_s^*(j) V_{ij} \psi_m(i) \psi_n(j) \, d\tau_i \, d\tau_j \tag{2.8}$$

and

$$\langle r |V|m\rangle = \int \psi_r^*(i) V_i \psi_m(i) \, d\tau_i \tag{2.9}$$

Using second-quantised formalism, and defining $\eta_k^+$ and $\eta_k$ as the creation and annihilation operators respectively, we write

$$H_0 = \sum E_m \eta_m^+ \eta_m \tag{2.10}$$

and

$$H_1 = \sum \langle rs |V| mn\rangle \eta_r^+ \eta_s^+ \eta_m \eta_n - \sum \langle r |V|m\rangle \eta_r^+ \eta_m \tag{2.11}$$

The summation on the right hand side of equation (2.11) is over all distinct matrix elements, where
\langle vs | \nu | \eta m \rangle \equiv \langle sr | \nu | \eta m \rangle \\
but \langle vs | \nu | \eta m \rangle \text{ is distinct.}

We shall be mainly concerned with the case of the groundstate \( \Phi_0 \) of the model Hamiltonian \( H_0 \). We suppose that \( H_0 \) has a non-degenerate ground state \( \Phi_0 \) formed from the lowest \( A \) of the \( \psi_n \)'s. The set of states \( \psi_n \) forming \( \Phi_0 \) will be called unexcited states and all others will be called excited states. Since the ground state is assumed to be non-degenerate any other configuration \( \Phi \) of the system will contain particles in the excited states and a complete description of \( \Phi \) is obtained by stating which of the excited states are occupied and which of the unexcited states are left empty. In analogy with the hole theory of Dirac, an unoccupied unexcited state will be called a "hole". We shall call \( \Phi_0 \) the vacuum and the particles in the states not contained within \( \Phi_0 \) as "particles". A natural consequence of this description is that the main effect of Pauli's exclusion principle is automatically taken care of, for an unexcited state will be regarded as normally occupied and hence excluded for other particles unless a hole in that state is explicitly introduced. The operators \( \eta_k \) and \( \eta_k^\dagger \) are regarded as annihilation and creation operators respectively of a particle, while for a hole their roles are reversed. In
this terminology a Fermi sea of particles has a description as follows. The vacuum state \( \Phi_0 \) is the filled up Fermi sea, i.e., a configuration where all one-particle states with momentum less than or equal to the maximum Fermi momentum \( k_F \) are occupied and there are no particles with momenta outside the Fermi sphere. For this system, all one-particle states with momenta \( k \leq k_F \) are unexcited states, and those with \( k > k_F \) are excited states.

According to the adiabatic theorem of Gell-Mann and Low, \( \Psi_\alpha \) the lowest eigenstate of \( H \) is expressed in terms of the ground state wave function \( \Phi_0 \) of \( H_0 \) with the help of the relation, which in the notation of Goldstone is given by

\[
\Psi_\alpha = \lim_{\alpha \to 0} \frac{U_\alpha \Phi_0}{\langle \Phi_0 | U_\alpha | \Phi_0 \rangle} \quad (2.12)
\]

Where \( U_\alpha \) is written as

\[
U_\alpha = \sum_{n=0}^{\infty} (-i)^n \int H_1(t_1) H_1(t_2) \cdots H_1(t_n) dt_1 dt_2 \cdots dt_n \quad (2.13)
\]

with

\[
H_1(t) = e^{iH_0 t} e^{-iH_0 t} \alpha t \quad (2.14)
\]

The adiabatic theorem states that

\[
H \Psi_\alpha = (E_0 + \Delta E) \Psi_\alpha \quad (2.15)
\]
where
\[ H_0 \Phi_0 = E_0 \Phi_0. \] (2.16)

and
\[ \Delta E = \langle \Phi_0 | H_1 | \Phi_0 \rangle = \Delta t \frac{\langle \Phi_0 | H_1 U_\lambda | \Phi_0 \rangle}{\langle \Phi_0 | U_\lambda | \Phi_0 \rangle}. \] (2.17)

Using the series for \( U_\lambda \) in equation (2.13) we obtain, after carrying out the time integrations, the perturbation expansions of \( \Psi_0 \) and \( \Delta E \) with the help of equations (2.12), (2.13), (2.17). Each term in the expansion of \( \Delta E \) and \( \Psi_0 \) in powers of \( H_1(t) \) becomes sum of products of matrix elements of \( V \) and \( V \) interactions, \( \varepsilon^t \), \( \varepsilon^t \) and \( \eta^t \), \( \eta^t \). This is easily seen by first writing the expression of \( H_1(t) \) which is obtained from equation (2.11) by substituting \( \eta_r(t) \) for \( \eta_r \) where
\[ \eta_r(t) = \eta_r e^{-iE_r t}. \] (2.18)

The expression for \( H_1(t) \) then becomes
\[ H_1(t) = \sum \langle rs | \nu | m \rangle \eta_r^+ \eta_s^+ \eta_m^+ \eta_n \ e^{i(E_r + E_s - E_m - E_n)t} - \sum \langle r | \nu | m \rangle \eta_r^+ \eta_m \ e^{i(E_r - E_m)t}. \] (2.19)
Fig. 1

Fig. 2

Fig. 3.

(a)

(b)

(c)

(d)

(e)

Fig. 4.
The different terms in equation (2.19) as well as those appearing in the different terms in the expansion of $\Psi_0$ and $\Delta E$ in powers of $H_1(t)$ can be represented by Feynman diagrams of $V$ and $V'$ interactions. Thus, one can as well obtain the required expansion for $\Psi_0$ and $\Delta E$ by writing down all possible graphs that may appear in the respective expansions. These graphs may be drawn and their contributions may be calculated with some suitable set of conventions as is done in field theories. We shall follow Goldstone in our approach.

Increasing time axis is drawn upwards from below. A particle line corresponding to a particle in the excited state is drawn by a line in the increasing direction of time, i.e., by an arrow pointing upward. Similarly, a particle in the unexcited state is represented by a line in the backward direction of time, i.e., by an arrow pointing downward. In the graphs $V'$-interactions are represented by dotted lines and $V$-interactions by dashed lines. All the interaction lines are drawn horizontally.

With these conventions, the matrix element corresponding to fig. 1 will be $\langle n|\Psi|m\rangle$ in which all the stable states $|m\rangle$, $|n\rangle$, $|r\rangle$, $|s\rangle$ are excited states. If we have initially one unexcited state $|n\rangle$, the matrix element will be represented by the fig. 2. A matrix element $\langle r|V|m\rangle$ will be represented by fig. 3 in the case of scattering of a particle between two unexcited states $|m\rangle$ and $|r\rangle$ due to a $V$-int
interaction. In this case the scattering is permitted only if a hole is already present in the state $|m\rangle$, otherwise such a graph is disallowed by exclusion principle. We can give many more examples like these. There is another class of graphs involving particle in the unexcited states in which the particle remains in its state after the interactions. Such particles are called by Goldstone "passive unexcited particles", and are represented by closed loops termed "bubbles". Some graphs involving "bubbles" are shown in fig. 4. Fig. 4(a) gives a diagonal matrix element of $V$ interaction in the unexcited state $|n\rangle$, i.e., $\langle n |V| n \rangle$. Similarly, fig. 4(b) gives the diagonal matrix element of interaction $\langle m |V| m \rangle$. Fig. 4(c) is the exchange graph of fig. 4(b). Fig. 4(d) and its exchange, fig. 4(e) represent the interaction of a passive unexcited particle with a particle in the excited state.

Over and above the first order terms, there will be terms of higher orders in $V$ and $\nabla$ interactions arising from higher order terms in $H_1(t)$ present in the expansion of $U_q$ in equation (2.13). There may be two distinct parts in a higher order diagram. The part of a graph which is completely disconnected from the rest of the graph and has no external lines attached to it is called an "unlinked part" and a graph which
has no unlinked part is called "linked graph". The unlinked parts of a graph represent disconnected vacuum processes. In figs. 5 the unlinked parts give first and second order vacuum processes respectively. If we consider all the terms in the expansion of $U_d$ in equation (2.13) we can split the linked and unlinked parts into two factors, one of which is the sum of all orders of linked diagrams and the other is the sum of all orders of vacuum processes. So the total transition amplitude for going from state $\Phi_1$ to $\Phi_2$ will be given by

$$\langle \Phi_2 | U_d | \Phi_1 \rangle = \langle \Phi_2 | R_d | \Phi_1 \rangle \langle \Phi_1 | U_d | \Phi_0 \rangle$$

where $\langle \Phi_1 | U_d | \Phi_0 \rangle$ is the vacuum-expectation value of $U_d$ while $\langle \Phi_2 | R_d | \Phi_1 \rangle$ is represented by connected graphs of scattering process only.

We can now write down the expansion of $U_d \Phi_0$ or $\Psi_0$ and $\Delta \mathcal{E}$ in terms of Feynman graphs. The vacuum $\Phi_0$ is not drawn in the graph, so that there will be no free lines at the bottom of the graphs appearing in the expansions of $\Psi_0$ or $\Delta \mathcal{E}$. Each graph will consist of a number of open loops of particle or hole lines, closed loops etc. From the analysis of the products of operators by Wick's algebra we have the following rule for the graphs appearing in $U_d \Phi_0$ and $\Delta \mathcal{E}$. For each graph multiply the $\mathcal{V}$ and $\mathcal{V}'$-matrix elements as they
appear in the graph and the $e^{i\hat{E}_t}$ and $e^{\hat{A}_t}$ factors and a factor $(-1)^{h+l}$ where $h$ is the number of internal hole lines and $l$ the number of closed loops. A passive unexcited particle loop as in fig. 4(a) contributes a plus sign, counting as one hole line and one closed loop, while fig. 4(b) has a minus sign having two hole lines and one closed loop. Each $\mathcal{V}$ matrix element has a minus sign attached since it occurs with a minus sign in $H_1$. There will be creation and annihilation operators corresponding to particle or hole lines at the end of each open loop. Finally, the time integrations are carried out. For labelling the graphs we ignore the Pauli exclusion principle in the intermediate states. The major effects of exclusion are already taken into account by the 'hole' picture described before. The rest must not be included. In fact all graphs which contradict the exclusion principle are exactly cancelled by their exchange graphs.

From equation (2.20) and the discussions following it, it is easily seen that after time integrations have been carried out the expansion of $\Psi_0$ given by equation (2.12) is that obtained by applying the rules of preceding paragraph only to the sum of all the linked graphs of $U_\tau \Phi_0$. This is because the other factor in the numerator of equation (2.12)
arising from unlinked graphs of $U_{d}\Phi_{0}$ is exactly cancelled out by the vacuum amplitude factor $\langle \Phi_{0} \mid U_{d} \mid \Phi_{0} \rangle$ already present in the denominator of the expression (2.12) for $\Psi_{o}$ as given by the adiabatic theorem. The final form of $\Psi_{o}$ can thus be written as

$$\Psi_{o} = \lim_{\xi \to 0} \sum_{L} \frac{1}{E_{o} - H_{o} + i\xi} H_{1} \frac{1}{E_{o} - H_{o} + i(n-1)\xi} \cdots \frac{1}{E_{o} - H_{o} + i(1)\xi} H_{1} \cdots \frac{1}{E_{o} - H_{o} + i\xi} H_{1} \frac{\Phi_{0}}{\Phi_{0}} (2.21)$$

where $\sum_{L}$ means that the terms are to be enumerated by the linked graphs only. This equation gives the "Linked cluster expansion" of $\Psi_{o}$. $\Phi_{0}$ cannot occur as an intermediate state in a linked graph as the part of the graph below that intermediate state would be an unlinked part. Since we have assumed the ground state $\Phi_{0}$ to be non-degenerate, all the intermediate states have energies greater than $E_{o}$. The limit in equation (2.21) can be taken by putting $\xi = 0$. Thus we can rewrite the expansion (2.21) as

$$\Psi_{o} = \sum_{L} \left( \frac{1}{E_{o} - H_{o}} H_{1} \right)^{n} \frac{\Phi_{0}}{\Phi_{0}} (2.22)$$

The linked cluster expansion for the energy shift $\Delta E$ can similarly be obtained from equation (2.17) and written as

$$\Delta E = \sum_{L} \langle \Phi_{0} \mid H_{1} \left( \frac{1}{E_{o} - H_{o}} H_{1} \right)^{n} \Phi_{0} \rangle (2.23)$$
where now $\sum$ means summed over all connected graphs leading from vacuum to vacuum, i.e. from $\Phi_0$ to $\Phi_0$, with no external lines in the graph.

It may be noted here that the energy denominators appearing in equations (2.22) and (2.23) are the differences between the model energies of the ground state and intermediate states which are the algebraic sums of single particle energies.

It was mentioned before that the exclusion principle is to be ignored while labeling the graphs, because all the graphs which violate the exclusion principle are exactly cancelled by their exchange graphs. But this is true as long as all the graphs as well as their exchanges are included in the summation. In the linked cluster expansions, however, this condition is not satisfied. For example, after removing the unlinked graphs, one removes fig.6(a), and is left with fig.6(b), which contains the strange feature of two particles in the same state $|m\rangle$ violating the Pauli principle in the intermediate state. Thus, in the linked cluster expansion, i.e., after removal of disconnected vacuum graphs, exclusion principle no longer holds in the intermediate states and one can have equally well two particles in a normally empty state and two holes in a normally occupied state and that there will
no longer be any cancellation of exclusion principle violating graphs.

The choice of single Particle Potential $V$

The energy $E = E_0 + \Delta E$ and the wave function $\Psi_0$ correspond to an exact solution of a many-body problem of a nucleus in its ground state, where $E$ and $\Psi_0$ are related by the Schrödinger equation (2.15), and $\Psi_0$ and $\Delta E$ are given by equations (2.22) and (2.23) respectively. It should be noted that equations (2.22), (2.23) and (2.16) constitute a solution of the many-body problem regardless of the choice of the single particle potential $V$, so that one can define $V$ in some suitable manners to serve different purposes. However, the expansions of $\Psi_0$ and $\Delta E$ are in the form of infinite series in powers of matrix elements of $V$ and $V'$ and those expansions are meaningful only when they are convergent and it is only then $E = E_0 + \Delta E$ and $\Psi_0$ correspond to a physical solution of a many-body problem. So, one possible way of removing the arbitrariness of $V$ will be to choose $V$ in such a way so as to make those expansions rapidly convergent such that a first few terms in the expansions need only be considered. By suitable choices of $V$ we can arrive at Hartree-Fock and Brueckner methods.
Hartree-Fock method

We define $V$ as given by

$$
\langle n | V | m \rangle = \sum_{n} \left\{ \langle n | V | m \rangle - \langle n | V | n \rangle \right\} \tag{2.24}
$$

where $|n\rangle$ is a state forming $\Phi_0$. The summation is over all unexcited states.

The states $\psi_n$ are determined by

$$(T + V)\psi_n = E_n \psi_n \tag{2.25}$$

Equations (2.24) and (2.25) are the Hartree-Fock self-consistent equations.

This definition ensures the complete disappearance of the $V$-interactions and the interactions with passive unexcited states from all graphs except the connected closed parts in figs. 4. Fig. 4(a) contributes $-\sum_{n} \langle n | V | n \rangle$ while figs. 4(b) and 4(c) contribute

$$
\frac{1}{2} \sum_{n} \left\{ \langle m_n | V | n \rangle - \langle m_n | V | n \rangle \right\} = \frac{1}{2} \sum_{n} \langle n | V | n \rangle \tag{2.26}
$$

when summed over all distinct possibilities.

Thus, to the first order in $V$,

$$
E^{(1)} = E_0 + \Delta E^{(0)}
= \sum_{n} \left\{ \langle n | T | n \rangle + \langle n | V | n \rangle \right\} + \frac{1}{2} \sum_{m,n} \left\{ \langle m_n | V | n \rangle - \langle m_n | V | n \rangle \right\} - \sum_{n} \langle n | V | n \rangle \tag{2.27}
$$
Fig. 7.

Fig. 8.
Since the H.F. definition of $V$ completely removes all the $V$-interactions and interactions with passive unexcited particles in all order, the higher order correction terms to $\Delta E$ is obtained by summing only over vacuum-vacuum linked diagrams with no $V$-interaction and interactions with particles in the passive unexcited states. Some such graphs are shown in fig. 7.

Thus we see that the H.F. definition of the single particle potential $V$ reduces greatly the number of terms to be summed over finally and as such it enhances the rapidity of convergence of the expansions (2.22) and (2.23) by bringing in the cancellation of a large number of diagrams. The discussion of H.F. approximation as made above also makes a good example to show the importance of the role of the single particle potential in bringing out the success of a many-body theory.
The many-body theory of nucleus, as developed by Brueckner and others, takes into account any number of interactions between two nucleons. In other words, it takes into account the diagrams of all orders connecting the same pair of particles at once. For example, when two particles scatter from the states $|m\rangle$ and $|n\rangle$ to the states $|p\rangle$ and $|q\rangle$ respectively, what one should take is the sum of all diagrams of the form as in fig. 8 at a time. These diagrams are called ladders. Whenever a diagram of two particle lines are connected by interaction lines, like the rungs of a ladder, with nothing else happening to the particles in between the interaction it will be called a ladder diagram of the two particles and the order of a ladder diagram will be one less than the number of rungs in it. The sum of all order ladder diagrams of two particles is called the reaction matrix of the two particles and may be written as

$$K = \sum_{n=0}^{\infty} v \left( \frac{1}{E_{0} - H_{0}} v \right)^{n}. \quad (2.29)$$

A graph will be called irreducible if it does not contain ladders of type of fig. 8.

The nucleon-nucleon potential seems to have a repulsive core at small distances. For this $V$ it is clearly impossible to
Fig. 9.

Fig. 10.
choose \( \nu \) by the H.F. method, as the matrix elements of \( \nu \) will have infinite contributions from the core. Brueckner theory replaces \( \nu \) by a reaction matrix \( \mathbf{K} \). The eq. (2.29) may be regarded as the solution of the integral equation for the reaction matrix which is

\[
\mathbf{K} = \nu + \nu \frac{1}{E_0 - H_0} \mathbf{K} \quad (2.30)
\]

With \( \nu \) replaced by \( \mathbf{K} \), we shall get finite results even for interactions with repulsive cores. Thus, it is possible to define the single particle potential \( \nu \) in terms of \( \mathbf{K} \)-matrices in a manner analogous to that in the H.F. theory. Also, \( \nu \) can be chosen in such a manner that when all the \( \nu \)-interactions are replaced by the \( \mathbf{K} \)-interactions, the resulting expansions of \( \Psi \) and \( \Delta \mathbf{E} \) in terms of \( \mathbf{K} \)-matrices are very rapidly converging.

Thus, in the Brueckner theory, in place of \( \nu \) and \( \nu \) in diagrams, we shall work with \( \mathbf{K} \) and \( \nu \) diagrams. In a diagram \( \mathbf{K} \)-interactions will be represented by wavy lines.

The diagonal elements of \( \mathbf{K} \)-interactions within the states of \( \Phi_0 \) will be represented as in fig. 9 and the corresponding matrix element is given by

\[
\langle mn | \mathbf{K} | mn \rangle = \langle mn | \nu | mn \rangle + \sum_{p, q} \langle mn | \nu | pq \rangle \frac{1}{E_0 - H_0} \langle pq | \mathbf{K} | mn \rangle \quad (2.31)
\]

Fig. 9 is actually the sum of diagrams of all orders as in fig. 10. The energy denominator \( E_0 - H_0 \) is given by
\[ E_0 - H_0 = E_m + E_n - E_i - E_j - \delta E \]  

(2.32)

To include the effect of all the other particles and holes present on a pair with K-interaction between them, we write the K-matrix equation as

\[ \langle b | K(\delta E) | m \rangle = \langle b | u | m \rangle + \sum \frac{\langle b | u | i \rangle \langle i | K(\delta E) | m \rangle}{E_0 - H_0} \]  

(2.33)

where K now depends on (\( \delta E \)) which is defined through

\[ \delta E = E_0 - E_0 - \sum E_i - \sum E_j - \delta E \]  

(2.34)

\( \delta E \) is the excitation energy of the complete intermediate state at the beginning of the interaction. The excitation energy is given by the sum of the energies of the occupied excited states minus the sum of the energies of the unexcited states in which there are holes. Thus \( \delta E = 0 \) for the K-diagram in fig. 9. We can finally write down the series expansions of \( \Psi_0 \) and \( \Delta E \) which we write as

\[ \Psi_0 = \sum \left( \frac{1}{E_0 - H_0} \right)^n \Phi_0 \]  

(2.35)

\[ \Delta E = \sum \left( \frac{1}{E_0 - H_0} \right)^n \Phi_0 \]  

(2.36)

where

\[ H_2 = \sum \langle rs | K(\delta E) | mn \rangle \eta_r \eta_s \eta_m \eta_n - \sum \langle r | V | m \rangle \eta_r \eta_m \]  

(2.37)
The summation convention in eq. (2.37) is the same as that in (2.11) and $\delta E$ of $K(\delta E)$ depends on the diagram of $K$-interaction considered in the summation. The summation in eqs. (2.35) and (2.36) are from $x = 0$ to $\infty$ and sum over $\Lambda$, means that the summation is restricted to the irreducible linked graphs only. From the definition of $K$-interaction it is clear that there cannot be a ladder of $K$-interactions.

Our task now is to choose $V$ in such a way that the expansions become useful, up to first order in $H_2$ we have

$$E^{(1)} = E_0 + \Delta E^{(1)}$$

$$= \sum \langle n | T | n \rangle + \frac{1}{2} \sum \left\{ \langle mn | K(0) | mn \rangle - \langle mn | K(\delta E) | mn \rangle \right\}.$$

(2.38)

We have to choose $V$ in such a way that it cancels the $K$-interaction with passive unexcited particles. However, unlike in the H.F. case, here the cancellation cannot be complete because of the dependence of $K$ on $\delta E$ which in many cases is not zero. The best we can do is to choose some average value of $\delta E$ appropriate to the matrix elements of $K$ to be evaluated and define $V$ in terms of $K$ for some mean excitation energy $\bar{\delta E}$ unless, of course, $\delta E = 0$. Thus one can have a definition of $V$ as

$$\langle r | V | n \rangle = \sum \left\{ \left| \langle n | K(\bar{\delta E}) | mn \rangle - \langle nr | K(\delta E) | mn \rangle \right| \right\}.$$

(2.39)
where $\delta E = 0$ when the states $|m\rangle$ or both $|v\rangle$ and $|m\rangle$
are unexcited states and $\delta E = \text{mean two particle excitation energy}$ where both the states $|m\rangle$ and $|v\rangle$ are excited states. Though one cannot be sure that this is the best definition of $V$, it seems to be a reasonably good definition, since it guarantees the smallness of higher order terms. Over and above the H.F. self-consistency, there is an additional requirement of self-consistency arising from the definition of the reaction matrix $K$ by eq. (2.30) which requires the whole of the energy spectrum $E_n$'s of eq. (2.25) to be known beforehand.

So we have here a self-consistency between $V$, $\psi_n$'s and $E_n$'s of the single particle problem. This new self-consistency is very important in Brueckner's theory. Since it is very difficult to work with such a self-consistency problem Brueckner and co-workers used an approximation which helped to overcome this difficulty. The energy differences appearing in the energy denominator are quite large. So they will correspond to quite small wavelengths. If the nuclear density is slowly varying over distances of this size, then the values of the excitation energies can be replaced by those of a spectrum appropriate to a uniform medium at the local density.
Brueckner chose to work with K-matrices in the coordinate space so that the approximation could be utilised and used the Fourier transform

\[(\vec{r}_1, \vec{r}_2 | K | \vec{r}_1', \vec{r}_2')\]

\[= \sum_{i, j, k, l} \psi_i^*(\vec{r}_1) \psi_j^*(\vec{r}_2) K_{ij, kl} \psi_k(\vec{r}_1') \psi_l(\vec{r}_2') \] (2.40)

Eq. (2.40) defines that coordinate space operator whose expectation value taken with respect to the eigenstates of the finite nucleus determines the interaction energies.

We notice in our discussions of H.F. and Brueckner theories that H.F. theory is only a particular case of Brueckner theory and H.F. theory is obtained from Brueckner theory by making crude approximations like replacing \(\Psi\) by \(\tilde{\Psi}\) and \(K\) by \(V\).

**No. 3. Review of some Fermi-Thomas models in Nuclear Physics**

It is well known that in the case of atoms there exists an approximation to the Hartree-Fock one when the terms in the energy expression are written as functions of density.
This approximation, the so-called Fermi-Thomas method, requires the density at any point to vary slowly over an electron wavelength. Though the Fermi-Thomas method is less accurate than the Hartree-Fock method, it has the advantage of being very simple and hence its importance. To get the Fermi-Thomas equation we write down the expression for the total energy for an atom

\[ E = C \int \rho^{5/3} d\mathbf{r} - e \int \rho \nabla \cdot d\mathbf{r} \]  

with \( C = \frac{3^2 (3\pi^2)^{2/3}}{10M} \), where \( \rho \) is the particle density and \( \nabla \) the total Coulomb potential at \( \mathbf{r} \). On minimizing \( E \) with respect to variations of the density \( \rho \), subject to the condition that the total number \( A \) of electrons shall remain constant, we get the equation for energy density as

\[ \frac{(3\pi^2)^{2/3}}{2M} \frac{t^2}{\rho^{2/3}} \rho = -e \nabla = -e\nabla_0 \]  

\( \nabla_0 \) is the Lagrange multiplier.

Combining equation (3.2) with Poisson's equation

\[ \nabla^2 \nabla = 4\pi e \rho \]  

we get the F.T. equation

\[ \nabla^2 (\nabla - \nabla_0) = \frac{4\pi e (2Me)}{3\pi^2 t^3} (\nabla - \nabla_0)^{3/2} \]
\[ E = \mu (V - V_0)^{3/2} \]  
\[ \mu = \frac{4\pi \varepsilon (2M_e)^{3/2}}{3\pi^2 k^3} \]

In case of atoms, i.e. for problems involving many electrons, this situation has been explored. Improvements with inclusion of exchange and surface corrections have also been made.

Situation is not so clear cut in case of nuclei. Several persons have applied the F.T. method to problems involving many nucleons. In most of these works the energy expression is written down more or less from semi-empirical considerations. Also, these authors mostly use trial density functions to minimise the energy of the nucleus which is expressed as a function of the density. The assumed density functions vary from Gaussian and Saxon-Wood to trapezoidal type profiles.

a) In the work of Gombas\[12\] the energy is written in the form

\[ E = \int \left\{ \frac{\xi(R)}{6} + \frac{k^2}{8m} \left( \frac{\nabla R}{R} \right)^2 \right\} dR \]  

where the first term in the integrand consists of the potential and kinetic energy densities in nuclear matter and the second term is the Weizsäcker correction to kinetic energy. By choosing a functional form for the density, the energy of
the nucleus can be minimised by varying parameters in the density function. Gombas tried several two-body potentials, but worked especially with Yukawa potentials. Saturation was obtained by exchange. The strength of the interaction was left as an adjustable parameter. Gombas was able to fit binding energies, including surface effects, over the entire range of nuclear masses fairly well with only one adjustable parameter. His density distributions, however, were unrealistic. He obtained Gaussian profiles for light and medium weight nuclei, and slightly flattened Gaussians for the heavy nuclei. The central density was an order-of-magnitude greater than observed.

b) Berg and Wilets\textsuperscript{13} considered the energy expression in the form

\[ E = \left\{ \mathcal{E}(\rho) + \frac{\xi k^2}{8M} \left( \nabla \rho \right)^2 \right\} d\vec{R} \] (3.7)

where they introduced a parameter $\xi$ multiplying the Weiszäcker energy term with values between $\frac{1}{2}$ and $\frac{1}{8}$ which depend on the potential one uses. Minimising the energy (3.7) with respect to $\rho$, subject to the condition that the total number of particles $A = \int \rho d\vec{R}$ remains fixed, Berg and Wilets got the differential equation

\[ -\frac{\xi k^2}{2M} \nabla^2 u + \frac{\partial \mathcal{E}}{\partial \rho} u = E_o u \] (3.8)
where \( u = \frac{1}{\sqrt{2}} \) and \( E_0 \) is the Lagrange multiplier.

To satisfy the saturation conditions they took the form of

\[
\mathcal{E}(\rho) = |E_0| \rho \left\{ -2 \left( \frac{\rho}{\rho_0} \right)^{\frac{\gamma}{\hbar}} + \left( \frac{p}{\rho_0} \right)^{2/\hbar} \right\}
\]

(3.9)

which provide analytical solutions for eq. (3.8). The density is given as

\[
\rho = \frac{\rho_0}{(1 + e^{x/\alpha})^n}
\]

(3.10)

with

\[\alpha = \frac{\kappa^2}{(8\pi M|E_0|)}\]

Vilets extended this method to the case of unequal numbers of neutrons and protons with Coulomb effects taken into account, the principle of the method being the same as in the previous one. If \( \lambda \) stands for \( n \) (neutrons) or \( p \) (protons), we can write, following Vilets the coupled differential equations corresponding to eq. (3.8) as

\[
-\frac{\mathcal{E} \kappa^2}{2M} \nabla^2 u_\lambda + \frac{\partial \mathcal{E}}{\partial \rho_\lambda} u_\lambda = E_0 u_\lambda
\]

(3.11)

The energy density \( \mathcal{E}(n, p) \) is assumed to be of the form

\[
\mathcal{E}(n, p) = \mathcal{E}(\rho) + k (\rho_n - \rho_p)^2 + V_C \rho_p
\]

(3.12)

The function \( \mathcal{E}(\rho) \), with \( \rho = \rho_n + \rho_p \), is taken equal to the \( \mathcal{E}(\rho) \) in eq. (3.9). The second term gives the nuclear symmetry energy and the third term represents the Coulomb energy.
Numerical integration of the coupled differential equations (3.11) leads to neutron and proton distributions which give quite good 90% - 10% fall-off distances. Since, however, these results were obtained in the semi-infinite approximation by putting \( \nabla^2 = \frac{d^2}{dR^2} \), we should be a little wary about them.

c) Skyrme\(^{14}\) started with the basic ideas of Brueckner's self-consistent nuclear model. After making a number of approximations he finally chose, in a more or less ad hoc manner, the fermion form of the energy density as

\[
\varepsilon = \rho E_0 \left\{ (1 - \frac{\rho}{\rho_0})^2 - 1 \right\} + \frac{1}{2} B (\nabla \rho)^2
\]  

(3.13)

where \( E_0 \) and \( B \) are constant.

Using the dimensionless variable \( \gamma = \frac{\rho}{\rho_0} \) and putting \( \frac{B \rho_0}{E_0} = \beta^2 \), and after minimizing the total energy subject to the normalising condition \( \rho_0 \int \gamma d^3 r = A \), he gets the differential equation

\[
2 \beta^2 \gamma^2 \nabla^2 \gamma = \frac{d}{d \gamma} \left( \gamma^3 - 2 \gamma^2 + \lambda \gamma \right)
\]  

(3.14)

where \( \lambda \) is the Lagrange multiplier.

Like Wilets, Skyrme also uses the semi-infinite approximation with \( \nabla^2 = \frac{d^2}{dR^2} \) which has the same defect.
d) Findler\textsuperscript{15}, in his work, assumed a static, charge independent, scalar meson potential. In his energy expression, he included the Fermi type kinetic energy along with its Weizsäcker correction and both the ordinary and exchange Coulomb energies. Like most other authors Findler also minimized the total energy which is written in terms of density. He chose the trial density function as a Gaussian function.

e) Of the more recent works, the semi-empirical statistical method of Wilets, with the use of trial nucleon densities has been used by Bodmer\textsuperscript{16} to investigate the nucleon density distributions and their relation with the semi-empirical mass formula. Ayres\textsuperscript{17} et al. assumed a trapezoidal density distribution and did not carry out the minimization of the energy expression completely. Rodberg and Teplitz\textsuperscript{18} started from the K-matrix theory of Brueckner and others. They used an amplitude and frequency modulated plane wave for the spatial part of the wave function written as

\[ \chi_i(r) = \int f(r) e^{i \mathbf{k}_i \cdot \mathbf{r}} \, dr \]  \hspace{1cm} (3.15)

Results obtained by minimising the energy expression using the trial function (3.15) and the "generalised Gaussian" density function

\[ f(R) = f_0 e^{-\left(\frac{R}{R_0}\right)^n} \]  \hspace{1cm} (3.16)

gave a binding energy which is too low, a radius which is too
small and a nuclear surface which is too diffuse.

In this work we have tried to develop a F.T. type method where Brueckner's K-matrix theory has been used. Our differential equation is obtained from a variational principle, and the energy is minimized fully with respect to all arbitrary parameters that enter through the boundary conditions.
CHAPTER II

The Dirac density matrix

1. It has been realised for some time that the Dirac density matrix can be used quite successfully to many-fermion ground state problems. It also provides a tool for improved formulations of the Fermi-Thomas method.

Let \( \psi_i(r) \), where \( i = 1, 2, \ldots \), be a complete set of orthonormal single-particle wave function in some potential \( \phi(r) \) as yet unspecified. Then the density matrix for the system is defined as

\[
\rho(r_1, r_2) = \langle r_1 | \rho | r_2 \rangle = \sum_S \psi^*_S(r_1) n_S \psi_S(r_2)
\]

where \( n_S \) is the number of particles occupying the state \( S \).

In consequence of the exclusion principle the eigenvalues of the \( n_S \) are 0 and 1 and so the matrix \( \rho \) satisfies

\[
\rho^2 = \rho
\]

and

\[
\text{trace} \rho = A
\]

is the total number of particles in the system.

Usually we deal with particles interacting by two-body potentials and the energy \( E \) of the system, with the above wavefunctions, is calculated as
where $H$ is the true Hamiltonian of the system. Then $f(\vec{r}, \vec{r}')$ is to be adjusted, subject to (1.2) and (1.3), so as to minimize $E$, and this can be done either by variation of the auxiliary potential $\phi$ or directly by variation of $f(\vec{r}, \vec{r}')$. Several authors have used the density matrix to give better theoretical basis to the F.T. method and to improve corrections like the inhomogeneity correction of Weizsäcker to the kinetic energy. Le Couteur started with the model Hamiltonian

$$H_m = T + \phi$$

(1.5)

with $(H_m, \phi) = 0$ \hspace{1cm} (1.6)

where $T$ is the kinetic energy operator. By considering different possible forms of approximations for the density matrix, he showed that one could get the different terms like the Fermi kinetic energy, Weizsäcker correction to the kinetic energy etc. In fact he showed that the standard Weizsäcker term should be multiplied by a factor $\frac{1}{9}$. A factor of about $\frac{1}{8}$ had been earlier suggested empirically by Berg and Wilets on basis of numerical comparisons of the exact and F.T. kinetic energies for some models.

2. A useful criterion to judge the merits of a F.T. density
Fig. 11. Comparison of density matrices for Rb$^+$ for $r = 1$ atomic unit. Curve a for statistical and curve b for Hartree-Fock density matrices are taken from Fröman. Curve c corresponds to the modified statistical approximation used in the present work.
matrix is to compare it with the Hartree-Fock density matrix, if and when available. Fröman\textsuperscript{21} made numerical comparison of the F.T. and H.F. density matrices for the case of $\text{He}^+$ ion (figs. 11 & 12). His statistical density matrix did not produce the violent oscillations and anisotropy found in the case of the H.F. density matrix. In order to obtain the F.T. density matrix Fröman proceeded in the following way. For the uniform matter case the density matrix

$$
(\mathbf{r} | \rho | \mathbf{r}') = \sum_i \psi_i^*(\mathbf{r}) \psi_i(\mathbf{r}')
$$

is given by

$$
(\mathbf{r} | \rho | \mathbf{r}') = \frac{1}{(2\pi)^3} \int e^{i \mathbf{k} \cdot (\mathbf{r}' - \mathbf{r})} d^3 k
$$

$$
= \frac{1}{\pi^2 |\mathbf{r}' - \mathbf{r}|} \int_0^{k_F} \sin \left\{ k |\mathbf{r}' - \mathbf{r}| \right\} \frac{k}{k} dk
$$

$$
= \frac{3}{2} n \left[ \frac{\sin \xi - \xi \cos \xi}{\xi^3} \right]
$$

where

$$
\xi = (3 \pi^2 n)^{1/3} |\mathbf{r}' - \mathbf{r}| = k_F |\mathbf{r}' - \mathbf{r}|
$$

and

$$
n = 2 \left( \mathbf{r} | \rho | \mathbf{r}' \right)
$$

is the density of electrons of both spins.

No completely satisfactory generalisation of these formulae...
Fig. 12. Comparison of density matrices for Rb$^+$ for $r = 2$ atomic units. Curve a for statistical and curve b for Hartree-Fock density matrices are taken from Fröman. Curve c corresponds to the modified statistical approximation used in the present work.
to the case of non-uniform density is known. Fröman used eqs. (2.1), (2.2), (2.3) with \( n \) replaced by the average of the densities \( n(\vec{r}) \) and \( n(\vec{r}') \).

For the H.F. case,

\[
\langle \vec{r}^2 | f | \vec{r}' \rangle = \sum_{n} \sum_{l=0}^{n-1} \sum_{m=-l}^{l} \left\{ \frac{t_{n,l}(\vec{r})}{\vec{r}} Y_{l,m}(\theta, \phi) \right\} \left\{ \frac{t_{n,l}(\vec{r}')}{\vec{r}'} Y_{l,m}(\theta', \phi') \right\} ^{\ast}
\]

\[
= \sum_{n} \sum_{l=0}^{n-1} \sum_{m=-l}^{l} \frac{t_{n,l}(\vec{r})}{\vec{r}} \frac{t_{n,l}(\vec{r}')}{\vec{r}'} 2l+1 \frac{p_{l}(\cos \alpha)}{4\pi}
\]

where \( Y_{l,m} \) are the normalized surface harmonics and \( \alpha \) is the angle between the directions \((\theta, \phi)\) and \((\theta', \phi')\). Comparing eqs. (2.1) and (2.4) (see figs. 11 & 12) we see that the density matrices differ vastly from each other.

We could try to find a form of the density matrix for non-uniform density\(^{22}\). The idempotency condition (1.2) implies

\[
\frac{1}{2} n(\vec{r}) = \int \left| \langle \vec{r}^2 | f | \vec{r}' \rangle \right| ^{2} d^{3}r'
\]

so that \( \langle \vec{r}^2 | f | \vec{r}' \rangle \) must tend to zero as \( n^{\frac{1}{2}} \) in regions of low density. This suggests that (2.1) be replaced by

\[
\langle \vec{r}^2 | f | \vec{r}' \rangle = \frac{3}{2} \left( \frac{n(\vec{r})}{n(\vec{r}')} \right) ^{\frac{1}{2}} \frac{\sin \zeta - \zeta \cos \zeta}{\zeta^3}
\]

with \( \zeta = \int \frac{kd\vec{r}}{\vec{r}^2} \) (2.7)

where at each point the local value of the Fermi momentum \( k \) is used, and the integral is over the line joining \( \vec{r} \) to \( \vec{r}' \).
The change in the values of $k$ arises due to the non-uniform character of the system involved. From eq. (2.6) we can write

$$\langle \mathbf{r} | \varphi | \mathbf{r}' \rangle = \frac{3}{2} \left( n(\mathbf{r}) n(\mathbf{r}') \right)^{1/2} \frac{j_1(\xi)}{\xi}$$

(2.8)

where $j_1$ is a spherical Bessel function. We can easily see that putting $\xi = \int_{\mathbf{r}'}^{\mathbf{r}} k d\mathbf{r}$ means a shift in the positions of the zero of the density matrix and they come approximately to the right positions. The application of (2.6) to Föman's example is shown in figs. (11 & 12). Eq. (2.6) can be seen to supply the zeros and reproduce the oscillations of $\langle \mathbf{r} | \varphi | \mathbf{r}' \rangle$ as $\mathbf{r}'$ approaches the atomic nucleus. Of course it is not accurate to connect points on opposite sides of the nucleus by (2.6), because of the singularity of the Coulomb potential. We shall see in later chapters that the new form of density matrix will be of great use in determining the parameters in the F.T. energy expressions.
Nuclear Potential Energy

According to the K-matrix theory of Brueckner and others the potential energy arising from the nucleon-nucleon interaction is given by

$$\Delta E = \Delta E_{nn} + \Delta E_{pp} + \Delta E_{pn}$$  \hspace{1cm} (1.1)

where

$$\Delta E_{nn} = \frac{1}{4\pi} \sum_{n_i n_j} \int \phi_{n_i}^*(\vec{r}) \phi_{n_j}^*(\vec{r}') K_{s,e}(\vec{r}, \vec{r}, \vec{r}', \vec{r}') \phi_{n_i}^{*}(\vec{r}') \phi_{n_j}^{*}(\vec{r}') \, d^3r \, d^3r' \, d^3r \, d^3r'$$ \hspace{1cm} (1.1a)

$$\Delta E_{pp} = \frac{1}{4\pi} \sum_{h_i h_j} \int \phi_{h_i}^*(\vec{r}) \phi_{h_j}^*(\vec{r}') K_{s,e}(\vec{r}, \vec{r}, \vec{r}', \vec{r}') \phi_{h_i}^{*}(\vec{r}') \phi_{h_j}^{*}(\vec{r}') \, d^3r \, d^3r' \, d^3r \, d^3r'$$ \hspace{1cm} (1.1b)

$$\Delta E_{pn} = \frac{1}{4\pi} \sum_{h_i n_j} \int \phi_{h_i}^*(\vec{r}) \phi_{n_j}^*(\vec{r}') K_{s,e}(\vec{r}, \vec{r}, \vec{r}', \vec{r}') \phi_{h_i}^{*}(\vec{r}') \phi_{n_j}^{*}(\vec{r}') \, d^3r \, d^3r' \, d^3r \, d^3r'$$ \hspace{1cm} (1.1c)

where the $\phi$ are single-particle wave functions in the model potential and the subscripts $s,e$ and $t,e$ denote the singlet-even and triplet-even parts. By expanding each wave function pair $\phi_{h_i}^{*}(\vec{r}) \phi_{n_j}^{*}(\vec{r}')$ about the centre-of-mass of particles $\vec{r}$ and $\vec{r}'$ one can express $\Delta E$ in terms of the neutron and proton densities at the point $\vec{r}$, namely...
\[ f_n(\vec{R}) = \sum_i |\phi_{ni}(\vec{R})|^2; \quad f_p(\vec{R}) = \sum_i |\phi_{pi}(\vec{R})|^2, \]
\[ f = f_n + f_p \quad \text{(1.2a)} \]

and their derivatives,
where the centre-of-mass and relative coordinates are given by
\[ \vec{R}_c = \frac{1}{2}(\vec{r}_1 + \vec{r}_2), \quad \vec{r} = \vec{r}_1 - \vec{r}_2. \quad \text{(1.2c)} \]

If we assume that the K-matrix has the form
\[ K(\vec{r}_1, \vec{r}_1'; \vec{r}_2, \vec{r}_2') = \delta(\vec{R} - \vec{R}') K(\vec{r}, \vec{r}', \vec{R}), \quad \text{(1.3)} \]
and use the BGW approximation that at every point \( \vec{R} \),
\( K(\vec{r}, \vec{r}', \vec{R}) \) may be replaced by the value appropriate to uniform nuclear matter at the density \( \rho(\vec{R}) \), then
\[ K(\vec{r}_1, \vec{r}_1'; \vec{r}_2, \vec{r}_2') = \delta(\vec{R} - \vec{R}') K(\vec{r}, \vec{r}', \vec{R}). \quad \text{(1.4)} \]

We can write equations (1.1a, 1.1b, 1.1c) as
\[ \Delta E_{nm} = \frac{1}{4} \sum_{n_i, n_j} \int \phi_{ni}^*(\vec{R} + \frac{1}{2} \vec{r}) \phi_{n_j}^*(\vec{R} - \frac{1}{2} \vec{r}) K_{s,e}(\vec{r}, \vec{r}', \vec{R}) \]
\[ \int \phi_{ni}^*(\vec{R} + \frac{1}{2} \vec{r}) \phi_{n_j}^*(\vec{R} - \frac{1}{2} \vec{r}) \ d\vec{r} \ d\vec{r}' \ d\vec{R} \quad \text{(1.5a)} \]
\[ \Delta E_{p} = \frac{1}{4} \sum_{k_i, k_j} \int \phi_{k_i}^*(\vec{R} + \frac{1}{2} \vec{r}) \phi_{k_j}^*(\vec{R} - \frac{1}{2} \vec{r}) K_{s,e}(\vec{r}, \vec{r}', \vec{R}) \]
\[ \int \phi_{k_i}^*(\vec{R} + \frac{1}{2} \vec{r}) \phi_{k_j}^*(\vec{R} - \frac{1}{2} \vec{r}) \ d\vec{r} \ d\vec{r}' \ d\vec{R} \quad \text{(1.5b)} \]
Expanding the single-particle wave functions $\phi$ in equation (1.5a) we have

$$\Delta E_{nn} = \frac{1}{4} \sum_{n_i n_j} \left\{ \phi_{n_i}^*(\vec{R}) + \frac{1}{2} \phi_{n_i}^* \left( \frac{1}{2} \vec{r} \cdot \vec{\nabla} \phi_{n_i}^* \right) + \frac{1}{2} \phi_{n_j}^* \left( \frac{1}{2} \vec{r} \cdot \vec{\nabla} \phi_{n_j}^* \right) - \frac{1}{4} \phi_{n_i}^* \left( \frac{1}{2} \vec{r} \cdot \vec{\nabla} \phi_{n_j}^* \right) - \frac{1}{4} \phi_{n_j}^* \left( \frac{1}{2} \vec{r} \cdot \vec{\nabla} \phi_{n_i}^* \right) \right\} + \text{higher order terms} \right\} \cdot \frac{\hbar^2}{m^2}$$

(1.6)

Since the terms containing odd powers of $\vec{r}$ and $\vec{r}^*$ vanish on integration over all angles, eq. (1.6) becomes

$$\Delta E_{nn} = \frac{1}{4} \sum_{n_i n_j} \left\{ \phi_{n_i}^* \phi_{n_j}^* + \frac{1}{2} \phi_{n_i}^* \left( \frac{1}{2} \vec{r} \cdot \vec{\nabla} \phi_{n_i}^* \right) + \frac{1}{2} \phi_{n_j}^* \left( \frac{1}{2} \vec{r} \cdot \vec{\nabla} \phi_{n_j}^* \right) - \frac{1}{4} \phi_{n_i}^* \left( \frac{1}{2} \vec{r} \cdot \vec{\nabla} \phi_{n_j}^* \right) - \frac{1}{4} \phi_{n_j}^* \left( \frac{1}{2} \vec{r} \cdot \vec{\nabla} \phi_{n_i}^* \right) \right\} + \text{higher order terms} \right\} \cdot \frac{\hbar^2}{m^2}$$

(1.7)
We keep up to the 2nd derivative of $\phi$ and neglect the higher derivatives; the justification of this ad hoc procedure is in section (5).

Hence we have for $\Delta E_{\infty}$, keeping terms up to the 2nd derivative of $\phi$,

$$\Delta E_{\infty} = \frac{1}{4} \sum_{nij} \left\{ \phi_i^* \phi_j^* - \frac{r_i^2}{12} \nabla \phi_i^* \cdot \nabla \phi_j^* + \frac{r_i^2}{12} \phi_i^* \nabla^2 \phi_j^* \right\}$$

$$= \frac{1}{4} \int \left[ \frac{p_n^2(\mathbf{r})}{4\pi} \kappa_{s,e} d^3r d^3r' - \frac{1}{16} \left( \nabla p_n^2 \right)^2 \int (r_i^2 + r_i^2) \kappa_{s,e} d^3r d^3r' - \frac{1}{12} p_n \tau_n \int (r_i^2 + r_i^2) \kappa_{s,e} d^3r d^3r' \right] d^3\mathbf{r}$$

$$= \int \left[ - a_i^s p_n^2 + a_2^s \left( \nabla p_n \right)^2 + \frac{4}{3} a_3^s p_n \tau_n \right] d^3\mathbf{r}$$

where

$$a_i^s = - \frac{1}{4} \int k_{s,e}(\mathbf{r}, \mathbf{r}', \mathbf{r}) d^3\mathbf{r} d^3\mathbf{r}'$$

$$a_2^s = - \frac{1}{32} \int k_{s,e}(\mathbf{r}, \mathbf{r}', \mathbf{r}) r_i^2 d^3\mathbf{r} d^3\mathbf{r}'$$

and

$$\tau_n = \sum_{n_i} \left| \nabla \phi_i \right|^2 \approx \tau_0 \rho_n^{5/3}$$

$$\tau_0 = \frac{3}{5} \left( \frac{3}{8\pi} \right)^{2/3} \left( 2\pi \right)^2 = 5.73$$
Proceeding in a similar way we get the expressions for $\Delta E_{pp}$ and $\Delta E_{pn}$ also in terms of density and its derivatives. So we have

$$\Delta E_{nn} = \int \left[ a_1^s f_n^2 + a_2^s (\nabla f_n)^2 + \frac{4}{3} a_2^s f_n \tau_n \right] d\mathbf{R}$$  \hspace{1cm} (1.9a)

$$\Delta E_{bb} = \int \left[ - a_1^s f_p^2 + a_2^s (\nabla f_p)^2 + \frac{4}{3} a_2^s f_p \tau_p \right] d\mathbf{R}$$  \hspace{1cm} (1.9b)

$$\Delta E_{bn} = \int \left[ (a_1^s + 3a_1^t) f_n f_p + (a_2^s + 3a_2^t) \nabla f_n \cdot \nabla f_p + \frac{2}{3} (a_2^s + 3a_2^t) (f_n \tau_p + f_p \tau_n) \right] d\mathbf{R}$$  \hspace{1cm} (1.9c)

$a_1^s$ and $a_2^s$ are defined by equations (1.10a & b), and

$a_1^t$ and $a_2^t$ are as follows:

$$a_1^t = -\frac{1}{2} \int k_{t,e} \left( \mathbf{r}, \mathbf{r}', f \right) d\mathbf{r} d\mathbf{r}'$$  \hspace{1cm} (1.10c)

$$a_2^t = -\frac{1}{2} \int k_{t,e} \left( \mathbf{r}, \mathbf{r}', f \right) r^2 d\mathbf{r} d\mathbf{r}'$$  \hspace{1cm} (1.10d)

$$\tau_p = \sum_{k_t} \left| \nabla \phi_{p_k} \right|^2 \approx \tau_0 \phi_{p_k}^3$$

We have assumed in the above discussion that (with $\mathbf{r} \equiv x_1, x_2, x_3$)

$$\int x_i x_j k d\mathbf{r} d\mathbf{r}' = \int k x_i' x_j' d\mathbf{r} d\mathbf{r}'$$

$$= \frac{1}{3} \delta_{ij} \int k r^2 d\mathbf{r} d\mathbf{r}' = \frac{1}{3} \delta_{ij} \int r^2 k d\mathbf{r} d\mathbf{r}'$$  \hspace{1cm} (1.12).

Equations (1.9) are too cumbersome for practical use. To simplify them we assume that the ratio of neutron and proton densities is the same at all points in the nucleus.
\[ p_t(R) = \frac{2}{A} p(R) = \frac{1}{2} (1 - \epsilon) p(R); \quad p_n(R) = \frac{N}{A} p(R) = \frac{1}{2} (1 + \epsilon) p(R) \] (1.13a)

\[ \epsilon = 1 - \frac{2Z}{A} \] (1.13b)

where for stable natural nuclei \( \epsilon \) ranges from 0 to 0.22.

Introducing the quantities

\[ \alpha_1 = \frac{3}{4} (a_i^s + a_i^t); \quad \alpha_2 = \frac{3}{4} (a_i^s + a_i^t), \] (1.14a)

\[ \bar{\alpha}_1 = \frac{1}{4} (a_i^s - 3a_i^t); \quad \bar{\alpha}_2 = \frac{1}{4} (a_i^s - 3a_i^t), \] (1.14b)

we get the following expression for the nuclear part of the potential energy

\[ \Delta E = \int \left\{ - (a_1 + \epsilon^2 \bar{\alpha}_1) \rho^+ + (a_2 + \epsilon^2 \bar{\alpha}_2) (\nabla \rho)^2 \right\} \]

\[ + \frac{2^{11/3}}{3} \sum \left[ a_2 (\epsilon_+^{5/3} + \epsilon_-^{5/3}) + \bar{\alpha}_2 \epsilon(\epsilon_+^{5/3} - \epsilon_-^{5/3}) \right] \rho^{8/3} \right\} \mathrm{d} \mathbf{R} \] (1.15)

where \( \epsilon_{\pm} = 1 \pm \epsilon \)

**Coulomb potential energy**

We consider only the direct part of the Coulomb potential energy.
From eq. (1.13a)

\[ E_c = \frac{1}{2} \int \mathcal{V}_c(\vec{R}) \mathcal{P}(\vec{R}) d\vec{R} \]  \hspace{1cm} (1.17)

where the Coulomb potential given by

\[ \mathcal{V}_c(\vec{R}) = \frac{1}{4} e^2 \varepsilon_0^2 \int \frac{\mathcal{P}(\vec{R}')}{|\vec{R} - \vec{R}'|} d\vec{R}' \]  \hspace{1cm} (1.18)

satisfies the Poisson equation

\[ \nabla^2 \mathcal{V}_c(\vec{R}) = -4\pi \frac{1}{4} e^2 \varepsilon_0^2 \mathcal{P}(\vec{R}). \]  \hspace{1cm} (1.19)

**Kinetic Energy**

Only the F.T. expression for the kinetic energy is used,

\[ E_{\text{kin}} = \tau_0 \frac{k^2}{2m} \int \left( p_x^{5/3} + p_y^{5/3} \right) d\vec{R}. \]  \hspace{1cm} (1.20)

From eq. (1.13a)

\[ E_{\text{kin}} = \tau_0 \frac{k^2}{2m} \int \left( \varepsilon_x^{5/3} + \varepsilon_y^{5/3} \right) \mathcal{P}^{5/3} d\vec{R}. \]  \hspace{1cm} (1.21)

It might be thought that in a theory for natural nuclei the kinetic energy term should include effects arising from the surface. The most widely discussed term of this type is that
due to Weizsäcker but the work of various authors\textsuperscript{13,20} on this term suggests that it is not a very useful correction to the standard F.T. expression. (See end of this chapter)

**Total Energy Density**

We introduce a convenient unit $f_0$ of density and a dimensionless variable $\gamma$ such that

$$f = \gamma f_0$$  \hspace{1cm} (1.22)

Then, collecting various expressions, we get for the total energy

$$E_{\text{total}} = \int \mathcal{E}_\gamma d\mathbf{r}$$  \hspace{1cm} (1.23)

with

$$\mathcal{E}_\gamma = \left\{ \frac{3}{5} \alpha \gamma^{5/3} + \frac{3}{5} \beta \gamma^{5/3} - \frac{1}{2} \gamma \gamma^2 + \frac{1}{2} \left( \nabla \gamma \right)^2 + \frac{1}{2} \chi (R) \gamma \right\} \left[ (a_2 + e^2 \bar{a}_2) f_0^2 \right.$$  \hspace{1cm} (1.24)

$$\alpha = \frac{5}{3} \gamma_0^2 \frac{t^2}{2M} \frac{5/3}{2} \left( e_+^{5/3} + e_-^{5/3} \right) \frac{p^{-1/3}}{2 (a_2 + e^2 \bar{a}_2)}$$  \hspace{1cm} (1.25)

$$\beta = \frac{8}{9} \frac{\gamma_0}{2} \frac{5/3}{2} \frac{a_2 \left( e_+^{5/3} + e_-^{5/3} \right) + \bar{a}_2 \varepsilon \left( \varepsilon^+ - \varepsilon^- \right)}{2 (a_2 + e^2 \bar{a}_2)}$$  \hspace{1cm} (1.26)

$$\gamma' = \frac{\alpha_1 + e^2 \bar{a}_1}{a_2 + e^2 \bar{a}_2}$$  \hspace{1cm} (1.27)
The factor $2(\varepsilon_2 + \varepsilon_1^2)$ and the other numerical factors in the above equations have been chosen in order to have the simplest form for the differential equations later. It must be remembered also that $\alpha, \beta$ and $\gamma$ have weak density dependences which follow from definitions (1.10). Eq. (1.28) for $V_c(\vec{r})$ differs from the actual Coulomb potential (1.18) and (1.19) by a constant factor as well as in being expressed in terms of $\gamma$.

2. Discussion of the K-matrix quantities occurring in the energy expression

According to section 4 of BGW 8, the density dependence of the K-matrix arises mainly from the part depending on the hard core and may be written as

$$k = k_{\text{core}}(\rho) + k_a$$

with

$$k_{\text{core}}(\rho) = k_{\text{core}}(\rho_e)f(\rho),$$

where $\rho_e$ is the equilibrium density of nuclear matter and $f(\rho)$ is a function of the form $a/(1-b\rho^{\frac{3}{2}})$ in which constants depend on the space-spin character of the K-matrix.
Using this form of the K-matrices the quantities in 
eqs. (1.10) may be expressed as

\[ a_i^q = b_i^q + d_i f_i^q (\mathcal{P}) \]  

(2.3)

where \( q = s \) or \( t \), \( i = 1 \) or \( 2 \) and

\[ b_i^q = -\frac{1}{4} \int (K_{\alpha, c})_a \, d\tau d\tau' \; ; \; \; b_2 = -\frac{1}{32} \int (K_{\alpha, c})_c r^2 d\tau d\tau' \]  

(2.4)

\[ d_1^q = \frac{1}{4} \int (K_{\alpha, c})_c d\tau d\tau' \; ; \; \; d_2 = + \frac{1}{32} \int (K_{\alpha, c})_c r^2 d\tau d\tau' \]  

(2.5)

The attractive part \((K_{\alpha, c})\) of the K-matrix is essentially 
the attractive part of the nucleon-nucleon potential itself and 
is by far the largest contribution to the quantities \( a \).

It is thus seen that within the framework of the BGW theory 
and the present approximation the quantities that determine 
the energy are primarily the first and second moments of the 
K-matrices. The density dependence of the K-matrices arises 
primarily from the hard core effects and is relatively small.
The quantities \( a_i \) of (2.3) are monotonic weakly decreasing 
functions of \( \mathcal{P} \). It is possible to obtain the quantities 
\( b \) and \( d \) whenever K-matrices are given.

For studying the effects on the energy expressions the quan-
tities \( a_1, a_2, \bar{a}, \bar{a}_2 \) introduced in 
eqs. (1.14) are more
It is evident from eq. (1.15) that the effect of $a_1$ and $a_2$ appears only when $N \neq \frac{2}{3}$, and is a second order effect in the small parameter $\epsilon$. The more important parameters are $a_1$ and $a_2$. In particular, for the nuclear matter case these are the only parameters needed.

Kumar and Bhaduri\textsuperscript{23} considered the case $p_n = \frac{p_p}{2} = \frac{1}{2}p$ without any Coulomb field; hence in their case the expression for energy was

$$\Delta E = \int \left[ c f^{5/3} - a_1 f^2 + a_2 (rf)^2 + \frac{4}{3} a_2 r f \right] d\mathbf{r} \tag{2.6}$$

with $c = 3.6 \frac{E^2}{2M}$, and $f = \sum_i |\nabla^2 \Phi_i|^2 \cong 3.6 f^{5/3}$.

An estimate of $a_1$ and $a_2$ was made by determining their $b$-parts from the attractive parts of the potentials used in BGW calculations. The $f(f)$ part was taken from that given by BGW and finally the two $d$-parts were obtained by requiring that the nuclear matter be stable at $p_o = 0.2 f^{-3}$ with binding energy per particle of 15 Mev, the last two quantities being the results obtained by BGW in their more elaborate treatment. The results obtained were

$$a_1 = 476 - 90 f(p) \tag{2.7a}$$

$$a_2 = 158 - 47f(p), \quad f(p) = 0.58 \left(1 - 0.78 p^{5/3} \right) \tag{2.7b}$$
In our case, if we want to estimate all the four quantities, the situation is not as clearcut. However, the dominant b-parts of the quantities $\alpha_{s,t}^{b}$ are again determined quite easily from the potential given by BGW. To determine the d-parts we assume that they are proportional to the corresponding b-parts and use the estimates for $d_1$ and $d_2$ from (2.7) to get the four numbers $\alpha_{s,t}^{d}$. This is admittedly crude but the uncertainties occur only in the small density dependent parts where the total change from $0$ to $p_0$ is at most 30%. We have

\begin{align}
4a_1^s &\approx 1583 - 300 \, f_s(p) \tag{2.8a} \\
4a_1^t &\approx 955 - 180 \, f_t(p) \tag{2.8b} \\
4a_2^s &\approx 634 - 190 \, f_s(p) \tag{2.8c} \\
4a_2^t &\approx 204 - 61 \, f_t(p) \tag{2.8d}
\end{align}

From (2.8) and (1.14b)

\begin{align}
\bar{a}_1 &\approx -80 - 19f_s + 34f_t \approx -80 + 15f(p) \tag{2.9a} \\
\bar{a}_2 &\approx 1.5 - 11.9f_s + 11.4f_t \approx 1.5 - 0.5f(p) \tag{2.9b}
\end{align}
We now notice that the quantities \( \bar{a}_1 \) and \( \bar{a}_2 \) are small differences of two relatively large quantities. Hence the error in their determination, especially in determination of their density dependent part is likely to be very large. On the other hand one sees from (1.15) that it is actually the ratios

\[
\chi_1 = \frac{\bar{a}_1}{a_1}, \quad \chi_2 = \frac{\bar{a}_2}{a_2}
\]

that are important for the energy density. The values obtained here are

\[
\chi_1 \approx -0.2, \quad \chi_2 \approx +0.01
\]

Although these are rather uncertain estimates it is clear that their magnitudes are small. Since in the energy expression they are always multiplied by \( \varepsilon^2 \) their influence is further reduced. Hence we shall assume throughout this work that \( \chi_1 \) and \( \chi_2 \) are small constants. Density dependent effects arising from this source will always be negligible.

Assuming \( \chi_1 \) and \( \chi_2 \) as given, there will be three parameters in the energy expression (1.24), which may be taken as \( a_1, a_2, f_0 \) or \( \alpha, \beta, \gamma \). By requiring that the binding energy per particle be a minimum at the \( \rho_0 \) density \( f_0 \) of nuclear matter (condition of Hugenholtz and Van Hove), we get one relation between these three parameters, so that only two of them
remain independent.

If we know the equilibrium density and the binding energy of nuclear matter we can then find out $a_1$ and $a_2$ and vice versa. If we are given any K-matrix we can evaluate $a_1$ and $a_2$ since they are the first and second moments of the K-matrix, and thus determine the equilibrium density and binding energy. In the next section we are going to find the values of $a_1$ and $a_2$ using the K-matrices given in BGW.

3. $a_1$ and $a_2$ from BGW K-matrices

The tables of the K-matrices in BGW do not include that part of the contribution due to the hard core of the nucleus which comes from the surface of the core. This contribution is given by the first term on r.h.s. of eq. (3.2) in the approximate analytical expression of BGW.

Furthermore the tables cover a range of values of $r$ and $r'$ from 0.4 fm to a certain value; outside this range some approximations have to be used which will be explained as we go along.

The $a$ are given as follows:

\[ a_1^\prime = -\frac{1}{4}\int k_{\gamma' e} \, d^3 r \, d^3 r' = -2\int 2\pi^2 k_{\gamma' e} r^2 \, r' \, dr \, dr' \]  
\[ a_2^\prime = -\frac{1}{32}\int k_{\gamma' e} r^2 \, d^3 r \, d^3 r' = -\frac{1}{4}\int 2\pi^2 k_{\gamma' e} r^4 \, r' \, dr \, dr' \]  

(3.1a)  

(3.1b)
The values of $K$ given in the tables of BGW are upto $\nu = 1.2$ fm. So, we split up the integrals (3.1) each into two parts. One part ranges from the core radius 0.4 fm. to $\nu = 1.1$ fm, and the other is for $\nu > 1.1$ fm. We take the upper limit of the first part of the integral as 1.1 fm. instead of $\nu = 1.2$ fm. only for simplicity of calculations, so that we can use Simpson's rule for numerical integration. The error of course is very small.

For the $\nu > 1.1$ fm. part of the integrals (3.1) the singlet parts can be calculated just by using the approximate analytical expression for the $K$-matrix as given in BGW for singlet $s$-state

$$
\langle r'|K|r \rangle = -\frac{\delta(r'-r_c) \delta(r-r_c)}{(4\pi r_c)^2} \bar{\mathcal{G}}_o(r_c,r_c) - \left[ \delta(r-r_c) \nu_a(r') \frac{\bar{\mathcal{G}}_o(r'_c, r'_c)}{\bar{\mathcal{G}}_o(r_c, r_c)} + (r \leftrightarrow r') \right] + \nu_a(r) \frac{\delta(r-r'_o)}{4\pi r^2} \tag{3.2}
$$

where $\nu_a$ is the attractive part of the potential and $\bar{\mathcal{G}}_o$ is the $s$-state Green's function given approximately by

$$
\bar{\mathcal{G}}_o(r,r') \approx \frac{1}{rr'} \left[ \frac{-\frac{\alpha}{k}}{r-r'} \right] - \left[ \frac{-\frac{\alpha}{k}}{r+r'} \right] \quad \text{if } x = 1.07 \text{ fm}. \tag{3.3}
$$

For the triplet state the $K$-matrix has the same form if we assume only $s$-state interactions. Although this same method can be applied in the triplet cases, it is better to use the function $f(r) = \int k \, d^2r'$ for the range $\nu = 1.2$ fm. to $\nu = 2.0$ fm.
(\(f(r)\) being given in the tables within this range), while \(\int_{k_1}^{k_2} d^2 \vec{r}' d^2 \vec{r}''\) is calculated by the use of trapezoidal rule. The rest of the integral, i.e. \(\int_{\frac{1}{2}}^{\infty} K d^2 \vec{r}' d^2 \vec{r}''\) is calculated by putting in the approximate BGW expression (3.2) for the K-matrix. It is shown in BGW that the non-local K approaches the local potential \(V(r)\) for large values of \(r\). But, as Kumar and Bhaduri\(^{23}\) have shown by calculating \(J(K) = \int K(\vec{r}, \vec{r}') d^2 \vec{r}''\), the K-matrix is markedly non-local and is not approximated by the local potential \(V(r)\) until up to at least 1.5 fm. So, instead of considering only the local potential \(V(r)\), it is generally better to take expression (3.2) for calculations.

To find the values of the integrals between \(\gamma = 0.4\) fm. and \(\gamma = 1.1\) fm., we use Simpson's rule for two variables. In case of \(a_1^s\) and \(a_1^t\), the integrand is symmetric with respect to \(\gamma\) and \(\gamma'\) (3.1a) (since K is symmetric in \(\gamma\) and \(\gamma'\)).

Simpson's rule for two variables can be written as

\[
\int_{a}^{a+2h} \int_{a}^{a+2h} f(x,y) \, dx \, dy = \frac{h^2}{9} \left\{ f(a,a) + f(a+2h,a) + f(a,a+2h) + f(a+2h,a+2h) + 4 \left[ f(a+h,a) + f(a,a+h) + f(a+2h,a+h) + f(a+h,a+2h) \right] + 16 f(a+h,a+h) \right\}
\]

(3.4)

where \(h\) is the width of the interval.
In calculating $a^s_1$ and $a^t_1$ we have to find the value of the integral $\int_\infty^x k \, d^3r' \, d^3r$, where for the singlet case $x = 1.1 \text{ fm.}$ and for the triplet case $x = 2.0 \text{ fm.}$ Writing $a^\alpha_1$ as

$$a^\alpha_1 = b^\alpha_1 + d^\alpha_1 f_\alpha (\rho)$$

as in equation (2.3) and using eq. (3.2), with Gammel-Thaler potentials, we get with the help of equations (2.4) and (2.5)

$$b_1^\alpha = -\pi \int_\infty^x v_\alpha \, r^2 \, dr = -\pi \int_\infty^x \frac{v_\alpha}{\mu_\alpha} \, e^{-\mu_\alpha x} \, r \, dr$$

$$= -\pi \frac{v_\alpha}{\mu_\alpha} \left[ \left. \frac{x \, e^{-\mu_\alpha x}}{\mu_\alpha} + \frac{e^{-\mu_\alpha x}}{\mu_\alpha} \right] \right]$$

$$= -\pi \frac{v_\alpha}{\mu_\alpha} \left[ \left. \frac{x \, e^{-\mu_\alpha x}}{\mu_\alpha} + \frac{e^{-\mu_\alpha x}}{\mu_\alpha} \right] \right]$$

and

$$d_1^\alpha f_\alpha (\rho) = -\frac{1}{4} \left[ 1 \mathcal{D}_{(\rho_c, \rho_c)} + \int_\infty \frac{v_\alpha (\rho)}{\mathcal{G}_\alpha (\rho_c, \rho_c)} \, d^3r \right]$$

$$= -\frac{1}{4} \left[ \left. \frac{v_\alpha}{\mathcal{G}_\alpha (\rho_0 + \frac{\alpha}{k})} \right| \right]$$

As mentioned previously, for the triplet case of $a_1$ (i.e., $a^t_1$), we calculate

$$-\frac{1}{4} \int_{1.2}^{2.0} k \, d^3r' \, d^3r = -\frac{1}{4} \int_{1.2}^{2.0} f(\rho) \, d^3r = -\int_{1.2}^{2.0} f(\rho) \, r^2 \, dr$$

Between $\rho = 1.1 \text{ fm.}$ and $\rho = 1.2 \text{ fm.}$ by using the trapezoidal rule we find

$$-2 \int_{1.1}^{1.2} \frac{1}{2} \pi^2 \, k \, r^2 \, dr' = 7.48$$

(3.7)
For \( a_z \) we have the following expressions for the corresponding ranges of \( \gamma \):

\[
\beta_2 = - \frac{\pi}{8} \frac{V_{\alpha}}{M_{\alpha}} \int_0^\infty e^{-\mu \alpha r^3} dr
\]

\[
= - \frac{\pi}{8} \frac{V_{\alpha}}{M_{\alpha}} \frac{1}{\mu \alpha x} \left[ \frac{x^3}{\mu \alpha} + \frac{3x^2}{\mu \alpha} + \frac{6x^1}{\mu \alpha} + \frac{6}{\mu \alpha} \right]
\]

\[
\delta_2 \int_0^\infty \frac{1}{f(x)} dr = - \frac{1}{32} \left[ \frac{\gamma_c^2}{G_0(\gamma_c, \gamma_c)} + \int_0^\infty \frac{V_d(r) (r^2 + \gamma_c^2)}{G_0(\gamma_c, \gamma_c)} d\gamma \right]
\]

\[
= - \frac{1}{32} \frac{\gamma_c^2}{G_0} - \frac{\pi}{8} \frac{V_d \gamma_c^3}{\mu \alpha \left( \mu \alpha + \frac{\alpha}{\kappa} \right)} e^{-\frac{1}{2} \mu \alpha x + \frac{\alpha}{\kappa} \left( \gamma - \gamma_c \right)}
\]

\[
- \frac{\pi}{8} \frac{V_d \gamma_c}{\mu \alpha} e^{-\frac{1}{2} \mu \alpha x + \frac{\alpha}{\kappa} \left( \gamma - \gamma_c \right)} \left[ \frac{x^2}{\mu \alpha} + \frac{2x}{\mu \alpha} \left( \mu \alpha + \frac{\alpha}{\kappa} \right)^2 + \frac{2}{\mu \alpha} \left( \mu \alpha + \frac{\alpha}{\kappa} \right)^3 \right]
\]

(3.8a)

(3.8b)

For singlet case (\( a_z^s \)), \( x > 1.1 \) fm., and for triplet case (\( a_z^t \)) \( x > 2.0 \) fm.

Also, between \( \gamma = 1.2 \) and 2.0 fms., for triplet case,

\[
- \frac{1}{32} \int_{1.2}^{2.0} K r^2 d\gamma d\gamma' = - \frac{\pi}{8} \int_{1.2}^{2.0} f(r) r^4 dr
\]

(3.9)

and between \( \gamma = 1.1 \) and 1.2 fms., we find

\[
- \frac{1}{4} \int_{1.1}^{1.2} 2\pi^2 K r^4 d\gamma d\gamma' = 1.2 \text{ } \text{ } \text{ (3.10)}
\]

Putting \( \kappa \) in eqs. (3.4) as \( 1 \) fm. and using Gammel-Thaler potentials as given in BGW, we get
\( a_1^s = 239, \quad a_1^t = 197, \quad a_2^s = 149, \quad a_2^t = 65. \)

Using relations (1.14a), we finally get

\[ a_1 = 327 \text{ Mev} \cdot \text{fm}^3; \quad a_2 = 160 \text{ Mev} \cdot \text{fm}^5. \]

Moszkowski and Scott\(^{24}\) have carried out nuclear matter calculations in momentum space. These also involve the volume integral of the BGW K-matrix and so can be used to provide a desirable check on the above estimate of \( a_1 \).

To compare with Moszkowski and Scott's calculation, we start from their definition of \( K(\vec{p}, \vec{p}') \)

\[
K(\vec{p}, \vec{p}') = \int_{-\infty}^{+\infty} \frac{i}{(\vec{p}, \vec{p} + \vec{p}', \vec{p}')} d\vec{r} d\vec{r}'.
\]  

(3.11)

So,

\[
k(0, 0) = \int_{-\infty}^{+\infty} k(\vec{r}, \vec{r}') d\vec{r} d\vec{r}'.
\]  

(3.12)

Also,

\[
a_1 = -\frac{3}{16} \int_{-\infty}^{+\infty} k(\vec{r}, \vec{r}') d\vec{r} d\vec{r}'.
\]  

(3.13)

If we consider only the singlet part \( a_1^s \) of the K-matrix, we can write

\[
k_s(0, 0) = \int_{-\infty}^{+\infty} k_s(\vec{r}, \vec{r}') d\vec{r} d\vec{r}'
\]  

(3.14)

\[
(a_1)_s = -\frac{3}{16} \int_{-\infty}^{+\infty} k_s(\vec{r}, \vec{r}') d\vec{r} d\vec{r}'.
\]  

(3.15)
and have the relation

\[ K_s(0,0) = -\frac{16}{3} (a_1)_s = -4a_1^s. \]  (3.16)

\((a_1)_s\) is defined in a slightly different way from \(a_1^s\) in eq. (3.1a) in the sense that

\[ (a_1)_s = \frac{3}{4} a_1^s. \]  (3.17)

\((a_1)_s\) is of course the singlet part of \(a_1^s\).

Putting \(a_1^s = 239\), as found before, in eq. (3.16) we get

\[ K_s(0,0) = -956 \text{ MeV} \]  (3.18)

This value of \(K_s(0,0)\) is quite close to the value 1000 MeV calculated by Moszkowshi and Scott (see their fig. 8) and so provides a verification for the result obtained by us.

4. Condition of Hugenholtz and Van Hove

To determine the equilibrium density \(\rho_0\) and the binding energy per particle \(\lambda\) in nuclear matter, we make use of the Hugenholtz and Van Hove condition that the binding energy per particle in nuclear matter be minimum. So, we have

\[ \frac{d(\varepsilon/\rho)}{d\rho} = 0 \]  (4.1)

\[ \alpha, \quad \frac{d\varepsilon}{d\rho} = \frac{\varepsilon}{\rho} = \lambda \]  (4.2)
Using eqs. (2.6) and (4.2) we get for the nuclear matter

\[ C \rho^{2/3} - a_1 \rho + 4.8 a_2 \rho^{5/3} = \lambda \]  
(4.3a)

\[ \frac{5}{3} C \rho^{2/3} - 2a_1 \rho + 12.8 a_2 \rho^{5/3} = \lambda \]  
(4.3b)

Knowing \( a_1 \) and \( a_2 \) we can find \( \lambda \) and \( \rho = \rho_0 \) (equilibrium density).

Using the values of \( a_1 \) and \( a_2 \) obtained in section 3 of this chapter we get the values of \( \rho_0 \) and \( \lambda \) as

\[ \rho_0 = 0.066 \text{ fm}^{-3}, \quad \text{and} \quad \lambda = 1.6 \text{ MeV} \]

which are vastly different from the result obtained by Brueckner et al.

\[ \rho_0 = 0.2 \text{ fm}^{-3}, \quad \text{and} \quad \lambda = 15 \text{ MeV} \]

This discrepancy would seem to cast strong doubts on the validity of the simple energy formula

\[ E_{\text{HF}} = - a_1 \rho^2 + \frac{4}{3} a_2 \rho^{4/3} + a_3 (\nabla \rho)^2 \]  
(4.4)

which was suggested by the first two terms of a power series expansion, but we shall see that the matter can be put right by more careful definitions of \( a_1 \) and \( a_2 \).

We recall that eq. (4.4) for the nuclear matter case with \( N = Z \) is obtained by expanding the H.F. like energy expression (compare sec. 1).
\[ \mathcal{E}_{\text{int}} = \sum_{i,j} \int \phi_i^*(\mathbf{r}_i) \phi_j^*(\mathbf{r}_j) K(\mathbf{r}_i, \mathbf{r}_j ; \mathbf{r}_i', \mathbf{r}_j') \phi_i(\mathbf{r}_i') \phi_j(\mathbf{r}_j') \ d\mathbf{r}_i \ d\mathbf{r}_j \ d\mathbf{r}_i' \ d\mathbf{r}_j' \]  

(4.5)

where \( i \) and \( j \) are single particle space states and \( K \) is the effective interaction summed over spins, or in the notation of the previous sections of this chapter,

\[ K \equiv K(\mathbf{r}, \mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') = \frac{3}{4} (K_{s,e} + K_{t,e}) \delta(\mathbf{r} - \mathbf{r}') . \]  

(4.6)

The \( a \) in eq. (4.4) are defined by

\[ a_1 = -\frac{1}{4} \int K(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}' \]  

(4.7a)

\[ a_2 = -\frac{1}{32} \int K(\mathbf{r}, \mathbf{r}') r^2 d\mathbf{r} d\mathbf{r}' \]  

(4.7b)

\[ a_3 = a_2 . \]  

(4.7c)

Actually, we have a series in \( (k_F/\mu) \) which diverges for values usually involved (\( \mu \) is the inverse range of the effective potential). It is shown in the following section (sec. 5) that it is possible to give an approximate justification for the forms (4.4) and (4.7) without invoking the series expansion.

5. Justification of the approximate form of nuclear potential energy

\( ^{29} \)

(i) In terms of the single particle density matrix
\[ f \left( \vec{r}, \vec{r}' \right) = \sum_i \phi_i^* \left( \vec{r} \right) \phi_i \left( \vec{r}' \right) = f_p \left( \vec{r}, \vec{r}' \right) + f_n \left( \vec{r}, \vec{r}' \right) = 2 f_p \left( \vec{r}, \vec{r}' \right) \]  

(5.1)

where the subscripts refer to neutrons and protons.

The potential energy eq. (4.5) is written as

\[ \mathcal{E}_{pot} = \frac{1}{2} \int f \left( \vec{r}, \vec{r}' \right) f \left( \vec{r}_2, \vec{r}_2' \right) K \left( \vec{r}, \vec{r}_2 ; \vec{r}', \vec{r}_2' \right) \, d\vec{r} \, d\vec{r}_2 \, d\vec{r}' \, d\vec{r}_2' \]  

(5.2)

We discuss approximations to the density matrices in sub-section (ii) for nuclear matter and in sub-section (iii) for nuclei and show that (4.4) is obtained from (5.2). We shall see that the expressions for the \( a \)'s are similar in form to (4.7) but differ by significant numerical factors.

(ii) **Nuclear matter case ; coefficients \( a_1 \) and \( a_2 \)**

Since the density is uniform the gradient term in equation (4.4) vanishes and the problem is fully determined by the two constants \( a_1 \) and \( a_2 \). In this case

\[ f = \frac{2}{3 \pi^2} k_F^3 \]  

(5.3)

and

\[ f \left( \vec{r}_1, \vec{r}_1' \right) = f \left( \vec{r} \right) \]  

(5.4)

with

\[ f \left( \vec{r} \right) = \frac{3}{\chi^3} \left( \sin \chi - \chi \cos \chi \right) = \frac{3}{\chi} j_1 \left( \chi \right) \]  

(5.5)

\[ \chi = k_F \left| \vec{r}_1 - \vec{r}_1' \right| \]
and \( j_1(x) \) is the spherical Bessel function.

From (5.2) then

\[
E_{kxt} = \frac{1}{4} p^2 \int \int \left( \frac{1}{2} k_F |r - r'| \right) K(r, r') d^2 r d^2 r'
\]

(5.6)

since

\[
(\hat{r} - \hat{r}') = 2 (\hat{r} - \hat{r}')
\]

Although the power series expansion of \( f^2 \) inside the integral does not lead to rapid convergence, a fairly good representation can nonetheless be obtained by writing

\[
\frac{q}{\pi^2} j_1^2(\alpha) = \int \int \frac{2}{\pi} = \int (\alpha) = \beta - q \left( \frac{\alpha^2}{\pi} \right)
\]

(5.7)

provided \( \beta \) and \( q \) are properly chosen. This gives the following expressions for the \( a \)'s

\[
a_1 = - \frac{1}{4} \int k(\hat{r}, \hat{r}') d^2 r d^2 r'
\]

(5.8a)

\[
a_2 = - \frac{q}{32} \int k(\hat{r}, \hat{r}') r^2 d^2 r d^2 r'
\]

(5.8b)

In order to make a proper choice of \( \beta \) and \( q \), let us consider a local \( s \)-state potential of the form

\[
k(\hat{r}, \hat{r}') = \nu(r) \frac{\delta(r - r')}{4\pi r^2}
\]

(5.9a)

\[
\nu(r) = - \nu_0 \frac{-Mr}{|Mr|}
\]

(5.9b)
\[ v(x) \]

In fig. (14) to show the integral of \( v(x) \) for \( x = 0 \) and the corresponding to the longest range potential used in NOW. On this scale the contribution from the other loops of the square of the Bessel function is not negligible. This is increased by the relatively large amplitude of the first loop, and also by the rapid decrease of the potential \( g(x) \) (fig. 19) and is the main reason for the approximation \( (5.7) \). Show this behaviour would be maintained even for non-local hard-core potentials. As we shall be able to replace the values of \( g(x) \) obtained below for those cases.
For this case (5.6) becomes

\[ E_{\text{pot}} = \rho^2 \int_0^\infty \frac{J_1(x)}{x} J_0(x) \, dx \]  

(5.10)

With \( x = k_F r \sqrt{x} \). In fig. (13a) we show the integrand of (5.7) for \( \mu = 1.44 \text{ fm}^{-1} \), corresponding to the longest range potential used by BGW. On this scale the contribution from all other loops of the square of the Bessel function is not visible. This is caused by the relatively large amplitude of the first loop, and also by the rapid decrease of the potential (fig.12b) and is the main reason for the approximation of (5.7). Since this behaviour would be maintained even for non-local and hard-core potentials we shall be able to use the values of \( p \) and \( q \) obtained below for those cases as well.

We set \( p = 1 \) in order that the formulae should be correct in the low density limit and choose \( q \) to fit the shape and area of the true integrand curve in fig. (13a). The optimum value is 0.6. For higher values of \( q \) disagreement at higher values of \( x \) becomes more pronounced (fig.13c) and for lower values of \( q \) the maximum of the approximate curve becomes more pronounced (fig.13d).

In section 3 of this chapter we have evaluated the integrals (5.8) with \( p = 1, \ q = 1 \) and found the values of \( a_1 \) and \( a_2 \) which give B.E. per particle = 1.6 Mev and \( f_0 = 0.066 \text{ fm}^{-3} \).
The diagram illustrates two functions, $g(x)\nu(x)$ and $\left[j_1^2(x) - g(x)\right]\nu(x)$, over the range of $x$ from 0 to 10. The graph shows the variation of these functions with $x$. The text accompanying the diagram discusses the implications of these functions in a theoretical context.
Fig.14. Schematic representation of the four points of the integrand in eqs. (III.4.5) and (III.5.2).
If instead we use $p = 1$, $q = 0.6$ in eqs. (5.8), we get

$$a_1 = 327 \text{ Mev-fm}^3, \quad a_2 = 96 \text{ Mev-fm}^5$$

These lead to a binding energy per particle of 9.4 MeV at the equilibrium density $\rho_0 = 0.176 \text{ fm}^{-3}$. These values are closer to the works of Brueckner, but it is not very useful to make any more detailed comparisons with the results of the Brueckner calculations, since as later work has shown, their results can change in a noticeable way with changes in their approximation procedures. In particular, there are difficulties in considering the density dependence of the potential energy in these theories as pointed out by Baker, Gammel, and Hill.

In a detailed discussion of approximations made in various $K$-matrix calculations, Brown et al. have concluded that these approximations tend to give overestimates of the actual value that may be expected. In particular, they estimate that Brueckner-Gammel calculations probably overestimate the binding energy by 2-4 MeV, because of the neglect of the effective mass introduced by off-the-energy shell propagation.

It is possible to use lower values for $p$ and $q$ and obtain curves which perhaps would not be in principle any worse than what we have shown; but as long as one remains fairly close to the correct curves, no substantial changes...
in the binding energy or equilibrium density can be obtained.

(iii) The case of Non-uniform Density: coefficient \( a_3 \)

To determine \( a_3 \) we need a generalisation of equation (5.4) for the case in which the Fermi-momenta at the points \( \vec{r}_i \) and \( \vec{r}_i' \) of \( \rho(\vec{r}_i, \vec{r}_i') \) are not the same. Only those forms of the density matrix need be considered which go over into equation (5.4) for uniform density. Thus the expressions for \( a_1 \) and \( a_2 \) derived in sub-section (ii) apply to all cases.

The usual generalisation of eq. (5.4) is

\[
\rho(\vec{r}_i, \vec{r}_i') = \rho(\vec{R}_i) f \left( \frac{k_F(\vec{R}_i)}{\vec{r}_i - \vec{r}_i'} \right) \quad \vec{R}_i = \vec{r}_i + \vec{r}_i' \quad (5.11)
\]

where values of \( \rho \) and \( k_F \) appropriate to the point \( \vec{R}_i \) (fig. 14) are taken. In chapter II we showed that for the atomic problems we can write down a better form of the density matrix as

\[
\rho(\vec{r}_i, \vec{r}_i') = \left[ \rho(\vec{r}_i) \rho(\vec{r}_i') \right]^{1/2} f \left( \int_{\vec{r}_i}^{\vec{r}_i'} k \, dr_i \right) \quad (5.12)
\]

where at each point the local value of the Fermi momentum \( k \) is used, and the integral is over the line joining \( \vec{r}_i \) to \( \vec{r}_i' \). For nuclear problems, however, this variation is negligible, and we can use the form
To see the change in the value of $a_3$ we use both the forms (5.11) and (5.13) of the density matrix. Substituting (5.11) and (5.13) separately in (5.2) and expanding only the densities around the common centre (fig. 14) we get on collecting all terms in $(\nabla \psi)^2$

$$a_3 = -g \int \left( \frac{1}{2} k_\perp | \overrightarrow{r} - \overrightarrow{r}' | \right) k(\overrightarrow{r}, \overrightarrow{r}') r^2 d^2r'$$

(5.14)

where for (5.11) $g = \frac{1}{48}$, and for (5.13) $g = \frac{1}{24}$.

These two expressions are quite different from (4.7c). The presence of the function $\int^2$ inside the integral may have been anticipated after the work of the previous sub-section. The power series expansion of wave functions does not permit any straightforward rearrangement into this form because of various ambiguities in higher orders and the approximation has to be understood in terms of the density matrix.

The factors $\frac{1}{48}$ and $\frac{1}{24}$ before the integral are also different from the factor $\frac{1}{32}$ in (4.7c). This may be roughly understood in the following way. Eq. (4.7c) is obtained by expanding the wave function along the lines $\gamma_1\gamma_2$ and $\gamma_3\gamma_2$; it covers the whole rectangle and gives a factor $\frac{1}{32}$. Eq. (5.14) with $g = \frac{1}{24}$ on the other hand is obtained from the density matrix (5.13) which also takes into account the variation in density over the whole rectangle but in a different way.
and the different factor $\frac{1}{24}$ is thus not surprising. If the density matrix (5.11) were taken it will give a factor $\frac{1}{48}$. The coefficient of the gradient term is thus sensitive to the way in which changes in density take place.

Eqs. (5.14) for $a_3$ seems to contain a complicated dependence on $\phi$ through $k_F(\rho)$. In order to see what it means we again consider the potential (5.9). Although this differs from the usual K-matrices in being local and in that the potential does not vanish at the core radius, these simplifications should not make any material difference. Eq. (5.14) now gives

$$a_3 = \chi a_2 \quad a_2 \text{ from (4.7 b)}$$ (5.15)

with

$$\chi = \frac{329}{9} \left[ \int_{0}^{\infty} x^{2}(x^{1/2}) e^{-\frac{\mu}{k_F} x^{3} dx} \right]$$

$$\int_{0}^{\infty} e^{-\frac{\mu}{k_F} x^{3} dx}$$ (5.16)

where $g$ takes values $\frac{1}{24}$ and $\frac{1}{48}$.

The numerator here is the Laplace transform of a product of Bessel-functions of order $\frac{3}{2}$ and may be taken from reference (31). We have

$$\chi = 96 g \left( \frac{\mu}{k_F} \right)^4 Q_1 \left( 1+\left( \frac{\mu}{k_F} \right)^2 \right)$$ (5.17)

where $Q_1$ is the Legendre function of the second kind. The maximum value of $\left( \frac{k_F}{\mu} \right)$ occurs for the singlet $s$-state in the Gammel-Thaler potential used by BGW and is nearly
unity. The least value is, of course, zero. Over most of the nucleus \(( k_F / \mu ) \approx 1\) and \(\lambda = 9.6g\). As \(k_F \to 0\) in the extreme limit, \(\lambda \to 1\) the value corresponding to \((4.7c)\), derived from expanding the wave function. The approach to the limit is slow so that \(\lambda\) deviates from its value of about 9.6g over a small part of the nucleus where the density approaches zero.

For the case of triplet K-matrices of BGW, which has the longest range, we get over most of the nucleus \(( k_F / \mu ) \approx 1.46\) and \(\lambda = 15.6g\).

By taking into account different ranges and magnitudes of singlet and triplet K-matrices of BGW, we get the values for \(a_3\) as

\[
a_3 = 72 \text{ Mev fm}^5 \text{ when } g = \frac{1}{24} \quad (5.18a)
\]

\[
a_3 = 36 \text{ Mev fm}^5 \text{ when } g = \frac{1}{48} \quad (5.18b)
\]

Thus the values obtained from the numerical K-matrices of BGW and the considerations of section (5) of this chapter are

\[
a_1 = 327 \text{ Mev fm}^3, \quad a_2 = 96 \text{ Mev fm}^5, \quad a_3 = 72 \text{ Mev fm}^5 \quad (5.19a)
\]

for \(g = \frac{1}{24}\)

and
\[ a_1 = 327 \text{ Mev fm}^3, \quad a_2 = 96 \text{ Mev fm}^5, \quad a_3 = 36 \text{ Mev fm}^5 \]

(5.19b)

for \( g = \frac{1}{48} \).

We shall see later in Chapter 5 that the result \( a_3 = 58.2 \text{ Mev fm}^5 \) which we get empirically falls neatly between the values 72 and 36, each of which corresponds to a plausible approximation to density matrix. This shows that the approximate representation of energy density proposed in this chapter is quite reasonable.

To show that in neglecting the Weizsäcker inhomogeneity contribution to the kinetic energy we were not very much wrong, following Le Couteur\(^{20}\), we write down the Weizsäcker contribution to the kinetic energy

\[
\frac{k^2}{72M} \left( \nabla \rho \right)^2 = \frac{k^2}{72M} \rho_0 \left( \nabla \rho \right)^2
\]

since \( \rho = \gamma \rho_0 \).

Now \( \frac{k^2}{M} = 42 \text{ Mev fm}^2 \).

So, at \( \rho = \frac{1}{2} \rho_0 \approx 0.1 \text{ fm}^{-3} \), we have

\[
\frac{k^2}{72M} \left( \nabla \rho \right)^2 = \frac{42}{7.2} \left( \nabla \rho \right)^2 \approx 6 \left( \nabla \rho \right)^2 \text{ Mev fm}^5
\]

This contribution is to be compared with \( a_3 = 58.2 \text{ Mev fm}^5 \) of Ch. V.

The 6 Mev fm\(^5\) makes only a small correction to the 58.2
Mev fm$^5$ so that our neglect of the inhomogeneity correction to the kinetic energy was not at all serious.
CHAPTER IV

SETTING UP OF THE DIFFERENTIAL EQUATIONS


Usually, the variational principle is written as

\[ \delta \int \left[ \varepsilon - \lambda \mathcal{F} \right] d\mathbf{R} = 0, \quad (1.1) \]

where the Lagrange parameter \( \lambda \) is determined from the constraint of the total number of particles

\[ A = \int \mathcal{F} d\mathbf{R} \quad (1.2) \]

It cannot be assumed that \( \mathcal{F} \) and \( \varepsilon \) automatically have correct behaviour at infinity. The equations obtained from (1.1) have no solutions with the exponential fall off appropriate for a quantum mechanical system. This is remedied usually by considering only the range of \( \mathbf{R} \) from the origin to the first zero of \( \mathcal{F} \) or by using some other type of cut-off.

By a more careful formulation of the variational principle we can obtain a consistent extension of the usual procedure. Considering only spherically symmetric forms of \( \mathcal{F} \), we want to minimise the integral

\[ I = \int_0^\mathbf{R} \left[ \varepsilon - \lambda \mathcal{F} \right] d\mathbf{R} \quad (1.3) \]
with respect to variations of \( f \) such that the value of \( f \) is not fixed for either of the end points 0 or \( R \). Furthermore the end point \( R \) itself is not fixed. The simultaneous minimum is obtained from the two equations

\[
\delta_f I = 0 \tag{1.4}
\]

\[
\frac{dI}{dR} = \left[ \xi - \lambda f \right]_{R=0} = 0 \tag{1.5}
\]

In the variational principle (1.4) one has to consider variations of \( f \),

\[
\delta f (\tilde{\mathbf{f}}) = \tilde{f}(\tilde{\mathbf{R}}) + \eta(\tilde{\mathbf{R}}), \quad \tag{1.6}
\]

where both \( \eta(0) \) and \( \eta(R) \) are arbitrary. Forming the integral \( I \) with \( \tilde{f} \) and minimising with respect to \( \eta \) in the usual way one obtains the result that the Lagrange equations

\[
\frac{\delta \xi}{\delta \tilde{f}} - \lambda - \nabla \left( \frac{\delta \xi}{\delta (\nabla \tilde{f})} \right) = 0 \tag{1.7}
\]

are satisfied provided the constants of integration are chosen so as to satisfy the condition

\[
\left[ \frac{\delta \xi}{\delta (\nabla \tilde{f})} - \eta \right]_{R=0} = 0 \tag{1.8}
\]

We require, for reasons of symmetry, that

\[
\nabla \tilde{f} = 0 \quad \text{at} \quad R = 0, \tag{1.9}
\]

and so with \( \xi \) given by (III. 1.24), (1.8) essentially
Further we note that eq. (1.5) is highly non-linear and presumably has several zeros, but the most natural zero is the one created by the vanishing of $p(\vec{R})$ itself. Hence from eqs. (1.5) and (1.10) we obtain the important result that the density distribution which properly minimises the integral (1.3) is the one which has a vanishing gradient at some point $\vec{R}$ and vanishes for $R \gg \bar{R}$. This boundary condition indirectly determines the density at the origin.

In this treatment we do not have the problem of interpretation connected with negative or infinitely increasing densities such as would occur if it were necessary to consider the solutions of eq. (1.7) throughout the whole space.

In the next section we discuss the particular forms of the Lagrange equations in the approximations (i) and (ii). These equations will be expressed in terms of the dimensionless quantity

$$\gamma = \frac{p}{\rho}.$$
\[ \nabla^2 y = x^2 y^{2/3} + \beta \gamma^3 - \gamma y + V_c + P, \]  \hspace{1cm} (2.1)\\

where \( V_c \) is the Coulomb potential with a different normalisation. It satisfies the Poisson equation

\[ \nabla^2 V_c = -Q \dot{y}, \]  \hspace{1cm} (2.2)\\

where from (III. 1.19), (III. 1.28)

\[ Q = \frac{\pi e^2}{2a_z} \varepsilon^2 \left( 1 + \varepsilon^2 z \right)^{-1}. \]  \hspace{1cm} (2.3)\\

Similarly, the quantity \( P \) in eq. (2.1) is the normalised Lagrange parameter

\[ P = -\frac{\lambda}{2a_z} \left( 1 + \varepsilon^2 z \right)^{-1}. \]  \hspace{1cm} (2.4)\\

Other symbols occurring here have been defined earlier in sections 1 and 2 of Chapter III.

On partially integrating the \( (\nabla y)^2 \) term in eq. (III. 1.24) and using eq. (2.1), one has

\[ E_{\text{total}} = 2 \left( a_z + \varepsilon^2 a_z \right) F_c^2 \int \left\{ 0.14 \gamma^3 - 0.125 \beta \gamma^3 - 0.5 \rho \gamma \right\} d\vec{R}. \]  \hspace{1cm} (2.5)\\

Eq. (2.5) holds only if \( y \) is a simultaneous solution of eqs. (2.1) and (2.2), subject to the conditions (1.9) and (1.10) together with \( y(\vec{R}) = 0 \).
(ii) An improved approximation to the general case.

As we have discussed before, a determination of density dependence directly from the BGW K-matrices is rather difficult. Therefore, we introduce a simplification in such a way that on the one hand it is still possible to make comparisons with the K-matrix quantities as calculated in sect. 2 of Chapter III and on the other hand the equations remain sufficiently simple so that one may utilise the results and experience of working in the approximation described in the previous subsection.

It was noticed in sect. 2 of Chapter III that $a_1$ and $a_2$ were monotonically decreasing functions of $y$. Instead of the forms indicated there, we shall assume forms for these such that the energy density in uniform matter is still given by an expression like (III. 1.24) with $\alpha, \beta$ and $\gamma$ still constants albeit modified.

We note that near $y = 1$ the density dependence of $a_1$ and $a_2$ can be represented by

$$a_1 = a_1^0 (1 - p y^{2/3}), \quad \bar{a}_1 = \bar{a}_1^0 (1 - p y^{2/3})$$

$$a_2 = a_2^0 (1 + q y^{-2/3}), \quad \bar{a}_2 = \bar{a}_2^0 (1 + q y^{-2/3})$$

with $a_1^0$, $a_2^0$, $p$ and $q$ constants. In order that these be decreasing functions of $y$, $p$ and $q$ should both be positive. On substituting in (III. 1.15) the energy density
takes the standard form

\[ \epsilon = 2a \left(1 + e^r \right) \frac{2}{\pi} \left( \frac{3\beta^3}{\xi_0^3} \right) \left( \frac{1}{2} \gamma^2 \right) + \left( \frac{1}{2} \frac{a_2(y)}{a^2} \right) \left( \frac{1}{2} \frac{a_2(y)}{a^2} \right) + E_c, \]  

(2.8)

where \( a, \beta \) and \( y \) are again constants given by eqs. (III. 1.25) to (III. 1.27) in which \( a_2 \) is replaced by \( a_2 \) and \( a_1 \) by \( a_1 \),

\[ a_1 = a_2 + \frac{3 \beta a_0}{\eta_0} \left( \frac{e^3}{\epsilon^3} + \frac{e^3}{\epsilon^3} \right), \]

(2.9a)

\[ \hat{a}_1 = a_1 - \frac{2}{3} \frac{a_2}{\eta_0} \left( \frac{e^3}{\epsilon^3} + \frac{e^3}{\epsilon^3} \right), \]

(2.9b)

and \( \hat{a}_1 \) and \( \hat{a}_2 \) are modified similarly. Now introducing a new variable \( z \) by the relation

\[ \left( \frac{d^2 z}{d\gamma} \right)^2 = \frac{a_2(y)}{a_2}, \]

(2.10)

and carrying out the variational procedure with \( \epsilon \) given by (2.8) one obtains the differential equations

\[ \nabla^2 z = \frac{d^2 y}{d\gamma} \left\{ q \gamma^2 + \beta \gamma^3 - y^2 + P + V_c \right\}, \]

(2.11)

\[ \nabla^2 V_c = - Q \gamma \]

(2.12)

where \( Q \) and \( P \) are again given by eqs. (2.3) and (2.4) with \( a_2 \) replaced by \( \hat{a}_2 \).

In the present case we have to solve three simultaneous equations (2.10), (2.11) and (2.12) instead of the two of the
previous subsection.

Strictly speaking eq. (2.10) must be solved in conjunction with (2.7) to obtain $y$ as a function of $z$. It is only when $y$ is obtained as a function $z$ that (2.11) and (2.12) give $z$ as a function of $R$. A further approximation has to be made because the form (2.7) is much too difficult for our purpose. Actually we assume

$$a_2(y) = \frac{u^2}{1 + s^2} \hat{a}_2,$$

(2.13)

because it enables (2.10) to be solved exactly and decreases with $y$ like (2.7) if

$$\frac{s}{1+s} \approx \frac{2q}{3(1+q)}.$$

The numerical method for the integration is given in the appendix.

We note that the approximation of the earlier section is the special case in which $u = 1$ and $s = 0$, $a_2 = \hat{a}_2$.

In order to justify the approximation introduced here we must show first of all that the standard energy density expression (2.8) is adequate. This approximation does not affect the Coulomb energy or the part depending on the gradient term, only the remaining part, that which is relevant to nuclear matter problem, is affected. If we consider the forms of density dependence of $a_1$ and $a_2$ given by
The effect of the density dependence of K-matrix on the energy density for nuclear matter. The values \( t = \hat{d}_1 = \hat{d}_2 = 0 \) (a) correspond to the standard approximation eq. (IV.2.16). (b) and (c) correspond to \( \hat{d}_1 = \hat{d}_2 = 0.2 \), \( t = 0.5 \) and \( \hat{d}_1 = 0.1 \), \( \hat{d}_2 = 0.2 \), \( t = 0.5 \), respectively in the Brueckner expression (IV.2.14). All expressions are constrained to have the same value at \( y = 1 \).
the BGW theory as in eq. (III. 2.7), then the energy expression relevant to nuclear matter ($\bar{\epsilon} = 0$) will be

$$\bar{\epsilon}_{nm}^B \left( \frac{3}{5} \gamma \frac{5}{3} + \frac{3}{8} \beta (1 + \bar{d}_2 f) \gamma \frac{7}{3} - \frac{1}{2} \gamma (1 + \bar{d}_1 f) \gamma^2 \right), \quad (2.14)$$

where

$$a_1 = \bar{a}_1 (1 + \bar{d}_1 f), \quad (2.15a)$$

$$a_2 = \bar{a}_2 (1 + \bar{d}_2 f), \quad (2.15b)$$

$$f = \frac{1}{1 - t \gamma \frac{4}{3}} \quad (2.15c)$$

and other definitions are as given previously with $a_2$ replaced by the constant $\bar{a}_2$.

This has to be compared with our standard form (2.8)

$$\bar{\epsilon}_{nm}^B \left( \frac{3}{5} \gamma \frac{5}{3} + \frac{3}{8} \beta \gamma \frac{7}{3} - \frac{1}{2} \gamma \gamma^2 \right), \quad (2.16)$$

where $a, \beta$ and $\gamma$ are given by eqs. (III. 1.25) to (III. 1.27) with $a_2$ replaced by the constant $\bar{a}_2$.

In our method we assume values of $a$ and $\beta$ and then calculate $\gamma$ in terms of them by requiring that $\bar{\epsilon}_{nm}$ and $\bar{\epsilon}_{nm}^B$ satisfy the Hugenholtz and Van Hove condition of sect. 4 of Ch. III. If we further require the right hand side of (2.14) and (2.16) to have the same value at $\gamma = 1$ (say) and therefore the same slope there, then there seems to be
very little difference between the two expressions (see fig. 15). In other words the approximation introduced by (2.6) and (2.7) is justified in as much as it represents the nuclear matter part of the problem.

The chief effect of the density dependence therefore manifests itself through the factor \((dy/dz)\) appearing in eq. (2.11). Thus, considerable simplification is achieved by assuming a form for the coefficient of the gradient term such that it simplifies the integration process and has the correct qualitative behaviour. Although the \((dy/dz)\) term in (2.11) influences the shape of the solution throughout the range \(y = 0\) to \(1\), the most significant changes occur near \(y = 1\). Our numerical integrations have verified that the surface thickness depends mainly on the value \(u^2/(1+s)\) of (55) at \(y = 1\), and that it is not helpful to vary \(u\) and \(s\) independently.

Since the variation in (2.15) between \(y = 0\) and \(y = 1\) is about 10% in \(a_1\) and 17% in \(a_2\) (see sect. 2 of Ch. III) we can fit (2.6) and (2.7) to this near \(y = 1\) taking \(p = 0.1\) and \(q = 0.1\) so that we have roughly from (2.9b) and (2.13)

\[
\frac{a_2(y=1)}{\hat{a}_2} \approx 0.88 \approx u^2.
\]  

(2.17)

It is thus seen that the density dependence given by the BGW K-matrix is too weak to make an appreciable effect on
the differential equation. Our arguments leading to this result are undoubtedly circuitous. This course was adopted chiefly because we wanted also to see the manner in which the density dependence of these quantities (provided it was strong enough) would make significant differences to the solution. The answer to this question is that the main effect is through the modification of the coefficient of the gradient term.

Finally we write down the energy expression in this approximation from (2.10), (2.11) and (2.12)

$$E(y) = 2\hat{\alpha}_2 (1 + \epsilon z_x) f_0^2 \left( \frac{3}{5} \beta \frac{y}{\gamma} + \frac{3}{8} \beta \frac{y}{\gamma} - \frac{1}{2} \frac{\gamma}{\gamma} + \frac{1}{2} \frac{y}{\gamma} V_z - \frac{1}{2} \frac{z}{\gamma} \right)$$  \hspace{1cm} (2.18)

and $\nabla^2 z$ is to be taken from (2.11) so that (2.18) reduces to (2.5) in the special case $y = z$. 
Fig. 16. Schematic representation of the variation in the nature of solutions $P + V_c(o)$. Curves a, b and c correspond to successively larger $P + V_c(o)$ but the same $y_o$. The optimum solution is tangential to the axis at $\bar{R}$, and lies between the curves a and b in the case given here. There might be more than one point like $\bar{R}$. In that case the curves with still higher values of $P + V_c(o)$ will also cross the axis.
Numerical Calculation

1. Procedure for Adjustment of Constants of Integration and Parameters

In our calculation we consider only the case in which \( y \) is spherically symmetric so that the integration over only one variable \( R \) is needed. The constant \( f_0 \) is chosen slightly greater than the central density of heavy nuclei which is also the assumed density of stable nuclear matter. As a result, the central value of \( y \), is expected always to have a value close to one. This choice of \( f_0 \) also provides an appropriate scale factor for the integration.

Since we have to solve two second order differential equations, we need four constants of integration. The numerical method is explained in the appendix. We start integrations from \( R = 0 \) where two of the constants are fixed because \( \frac{dy}{dR} = \frac{dV_c}{dR} = 0 \). One has thus to provide only the values \( y_0 \) and \( V_c(0) \) of the two functions at the origin. In fact, it is the combination \( (P + V_c(0)) \) which determines the solution once \( y_0 \) is given. With all other parameters fixed for a given \( y_0 \), the manner in which the solutions usually change with \( (P + V_c(0)) \) is shown schematically in fig. 16. Between the solution a which crosses the axis and the solution b which turns up without touching the \( R \)-axis
there must be a solution which is tangential to the axis at some point \( \tilde{R} \). This is the solution we search for. Since this solution provides a minimum of the energy, small deviations from exact contact cause only small changes in the energy. This has both advantages and disadvantages. On the one hand as far as energies are concerned we need not concern ourselves too much with obtaining exact contact and on the other hand just because we are close to a minimum and the differences are small the problem of discriminating between solutions belonging to different sets of parameters (especially different \( \epsilon \), with all others fixed) becomes very tricky. It may be noted in passing that occasionally as \((P + V_c(0))\) increases the curves may again cross the axis at a larger distance thus giving a proper solution for a higher value of \( A \) also.

In order to cover the whole periodic table the procedure is briefly as follows: The machine (IBM-1620, Fortran language programs) is given the numbers \( \varphi(0) \) and \( \beta(0) \) which are the values of \( \varphi \) and \( \beta \) for \( \epsilon = 0 \). It computes the value \( \varphi(0) \) from Hugenholtz-Van Hove condition. The relation is quite simply

\[
\varphi(0) = 0.8 \varphi(0) + 1.25 \beta(0).
\]  

(1.1)

Next one supplies the parameters \( \chi_1, \chi_2 \) and (also \( s \) and \( u \) of
eq. (2.13) if the approximation of sect. 4(ii) of Ch. IV is used) the machine then computes $a, \beta, y$ and $\epsilon$ for the given value of $\epsilon$. Finally the constants of integration $y_0$ and $(P + V_c(0))$ are specified the machine integrates the relevant equation till either $y$ crosses the $R$ axis or it turns up. The Coulomb potential $V_c$ and density $y$ are printed out for successive values of $R$ and in the final print among other things the average energy per nucleon, the corrected values of $P$ and $V_c(0)$ (see appendix) central density, and the mass number $A$ are printed out.

For each $y_0$, $P + V_c(0)$ is varied till a curve with $y$ tangential to the $R$ axis is found. In practice a given $y_0$ may produce such optimum curves for a small range of $A$ values because of the limited finesse required for fitting. For a given $A$ one then selects the $y_0$ for which the average energy per particle is the least. This achieves the minimisation with respect to the constants brought in by the boundary conditions and a graph of binding energy versus mass number is obtained. With each point on this graph are associated two numbers $y_0$ and $P + V_c(0)$ which give the minimum for this particular value of $A$.

For given $\gamma$, $\beta$, $x_1, x_2$, $s$ and $u$ we obtain for each value of $\epsilon$ a curve of binding energy versus $A$ as described in the last paragraph. We shall display these curves for $\epsilon = 0, 0.1, 0.17, 0.2$ etc. for some representative sets of parameters.
Fig. 17. The binding energy curve corresponding to parameters derived from BGW $\lambda$-matrices in density independent approximation. The points are from results of ref. 11. Note that the binding energy is in general two low.
An envelope of the minima of these curves, which will not actually be drawn on the figures, is to be compared with the experimental binding energy curve.

2. Discussion and results

(i) Density independent approximation

It has been shown in the previous section that the density dependence of K-matrices from BGW is so weak that it may be neglected with justification. If we require the binding energy of nuclear matter to be 15 MeV and its density $0.195 \text{ fm}^{-3}$ at equilibrium then we get, following Kumar and Bhaduri, but in the density independent approximation,

$$d = 0.9095, \quad \beta = 2.152 \quad (2.1)$$

The values of $x_1$ and $x_2$ were taken directly from the simple calculation of Ch. III Sect. 2, eq. (2.11). The curves obtained with this set of parameters for $\xi = 0, 0.1$ and $0.2$ are shown in fig. 17. The results of Brueckner, Lockett and Rotenberg are plotted for comparison. The fact that the point for Zr sits almost exactly on our curve has no particular significance. But together with the fact that the points corresponding to Ca and $0.16$ deviate from our curves in the expected direction it would seem to indicate that the present can be quite useful. We may not compare the magnitudes of the deviations in binding
energies for Ca\(^{40}\) and O\(^{16}\) because of the low mass numbers involved and also because in these nuclei both neutron and proton shells are closed. What is remarkable is that for values of parameters as determined in sect. 2 of Ch. III the results do give binding energies at all comparable to those from the calculations of Brueckner \(^8, 27\). The density distributions obtained by us in this case happen to be too diffuse at the surface. The fall off distances obtained by us vary from 3.0 fm. in light nuclei to 3.4 fm. in heavy nuclei. Furthermore, as might be expected, the densities obtained by us are flat and monotonic whereas those obtained by Brueckner, Lockett and Rotenberg show fluctuations characteristic of H.F. type calculations.

It was found that variation of the constant \(\beta\) only produced a variation in the equilibrium density at the centre while a variation in \(\alpha\) effectively moved the whole system of curves up or down in energy. No substantial change in the nature of the curve was noticed. In particular the reduction in binding energy per particle in going from mass numbers near the maximum (\(A \approx 80\)) to the highest masses (\(A \approx 230\)) is not nearly enough. In fig. 18 we present the results for \(\alpha(0) = 0.77\) and \(\beta(0) = 2.152\) which is adjusted to give right binding energy at the maximum. It is seen that the binding energy for heavy nuclei is excessive.
The binding energy curve with parameters adjusted to have nearly correct value at the maximum in density independent approximation. Note the excess binding for heavy nuclei. The choice of $x_1$ is not optimum but this has only second order effect on binding energy.
The parameters $x_1$ and $x_2$ cause only minor changes in the binding energy but they determine the most stable value of $\epsilon$ for a given $A$. The average energy discrimination between different $\epsilon$ values for the same $A$ is a small effect noticeable only in the third significant figure. Once the broad features of the binding energy curve are fixed by a choice of $\phi(0)$ and $\beta(0)$ the details of stability are adjusted by varying $x_1$ and $x_2$. In practice variation in $x_2$ are not significant and we have not tried too many values. Further, we search for values of $x_1$ and $x_2$ only in the vicinity of those given in eq. (III, 2.11). The influence of $x_1$ is best seen by noting the cross over points for curves belonging to different values of $\epsilon$. In fig.17 the cross-over of the curves for $\epsilon = 0.1$ and 0.2 is in the correct region (i.e. where it actually occurs experimentally) but when the value of $\phi(0)$ is changed to 0.77 the cross-over point changes in such a way that a lower value of $x_1$ was indicated. In fig. 18 curves corresponding to $x_1 = -0.1$ are shown. It is seen that even here the curve for $\epsilon = 0.17$ has more binding than the curve for $\epsilon = 0.2$ in a region where experimentally the situation is just the reverse. This indicates that a value of $x_1$ between 0.0 and -0.1 would be more appropriate.

Other calculations with the density independent approximation confirmed that (a) it was impossible to get the correct shape
Fig. 19. The binding energy curve in the density dependent approximation of Ch.IV. 2(ii). Parameters have been adjusted to give best agreement.
of binding energy curve by any adjustment of the parameters and (b) even for the best results in this respect the density distributions obtained were too diffuse — the fall-off distance varying from 3.0 fm to 3.5 fm as one goes from light to heavy masses.

(ii) The density dependent approximation

In fig. 19 we finally present the best binding energy curves we have been able to obtain. These were obtained in the density dependent approximation of Ch. IV, Sect. 2 (ii). The constants \( q(0), \beta(0), x_1 \) and \( x_2 \), \( s \) and \( u \) are adjusted for obtaining agreement with all three chief experimental quantities viz. the binding energies, neutron excess (cross-over points for curves with different \( \epsilon \) ) and density distributions. The values needed are

\[
q(0) = 0.875, \beta(0) = 2.15^2, x_1 = -0.04, x_2 = 0.01,
\]

\[
s = 0, \quad u = 0.7
\]

which imply

\[
y(0) = 3.39, \eta = 0, \beta = 0.24
\]

so that

\[
a_1 = 4.02 \left(1 - 0.24 y^{1/3}\right) \mu_N \rho_f^3 \text{MeVfm}^3; a_2 = 58.2 \mu_N \rho_f^5\]

which can be compared with the a priori values (III. 2.7).
Fig. 20. Representative density distribution for the case corresponding to fig. 19. Fall-off distance changes from 2.5 $f_{m}$ for light nuclei to 2.25 $f_{m}$ for heavy nuclei.
Fig. 21. Effective single particle potential $V_{eff}$ and Coulomb potential in a few typical cases. The graphs are for the following values: (1) $\xi = 0.1$, $A = 23$; (2) $\xi = 0.15$, $A = 104$; (3) $\xi = 0.2$, $A = 194$; (4) $\xi = 0.22$, $A = 232$. The effect of an increase in $\xi$ tends to make the potential only slightly less diffuse.
A comment regarding the role of the last two constants in (2.2) is needed. The value of \( u \) is very low compared to the value from the K-matrices (eq.(59)). Further, \( s = o = q \) is an extreme choice. Any finite value of \( s \) or \( q \) will do provided it is \( \ll 1 \). The effect of an increase in \( s \) tends to make the densities only slightly less diffuse. Actually the value of \( s \) that can be assumed should be much less than one, and therefore, the value of \( u \) as obtained here cannot be significantly increased by taking \( s \neq o \).

In fig. 20 we give density distributions for six representative masses for parameters given by (2.2). A tendency for the nuclei to become less diffuse with increasing \( A \) may be noted, the fall-off distances going from 2.5 fm to 2.25 fm. Also the heavy nuclei are very slightly hollow in the centre.

It is a comparatively simple matter to calculate the effective single particle potential, including the average Coulomb energy, for the last particle, once the density is known,

\[
V_{\text{eff}} = - \left( a'(0) \gamma^{2/3} + p \right) 2a_z f_0 .
\]  

(2.4)

We plot a few representative examples in fig. 21 together with the Coulomb potential obtained.
We have, in this thesis, developed a Fermi-Thomas type method and used it to calculate the binding energies and density distributions in nuclei for the whole range of mass values. In this work we were motivated by the following considerations. Instead of using the F.T. method as an empirical method we wanted to derive the quantities occurring in the energy density from a Hartree-Fock like theory, e.g., the K-metrix theory of Brueckner, which has a sound theoretical basis. Also, the binding energy and the density distribution were to be obtained by solving the differential equation obtained from a variational principle.

We find that by expanding each single-particle wave function pair \( \phi_1^{(1)} \phi_2^{(2)} \) about the centre-of-mass of particles \( \mathbf{1} \) and \( \mathbf{2} \) and keeping up to the 2nd order in \( \phi \) and \( \nabla \phi \) we can write down an expression for nuclear potential energy density in the simple form (4.4). Though the series does not converge, we can give a justification for the use of the simple form of energy density (4.4) with the help of the density matrix, some of whose structural properties we studied for the atomic case in CH.II getting very good agreements with those of exact Hartree-Fock atomic calculations. In CH.III
Sect. 5 these approximate forms of the density matrix were used along with local potentials, instead of the K-matrix, giving reasonable values for the parameters $a$. Though, in this way, the use of the energy expression (4.4) is very well justified, one may not use these values of the parameters $a$ as the starting point for an exact calculation due to the various approximations involved in evaluating the quantities $a$. Instead we determine $a_1$ and $a_2$ following the procedure of CH.III Sect. 2 in which case $a_3 = a_2$. We find (CH.V Sect. 2) that if we do not consider the density dependence of $a_1$ and $a_2$ it is impossible to fit both the densities and the binding energies throughout the periodic table. In particular the nuclear surface appears to be too diffuse and there seems no possibility of generating sufficient slope in the binding energy curve between medium and heavy masses. By considering the density dependence of $a_1$ and $a_2$ of the form of CH.IV Sect. 2 we get the right sort of changes and very good agreement with the experimental data is obtained. With parameters derived from BGW we obtain binding energies of about 6 MeV per nucleon in agreement with theirs, hence it is natural that when the parameters are adjusted to fit data as indicated above, the constants will not agree with those calculated from the K-matrix of BGW. This suggests that a calculation by the present method can be used to test whether for any given interaction potential a BGW type K-matrix calculation for nuclear properties would be likely to succeed. Apart from demonstrat-
demonstrating the feasibility of success in the other method our calculations will also provide the single particle effective potentials which would be convenient starting points for proper H.F. type calculations.

In this approximation only $a_1$ and $a_2$, the first and second moments of the K-matrix, and their density dependence are of importance. We find that the density dependence of the K-matrix of BGW is too weak and can be neglected. For obtaining agreement with experiment it is not only necessary to assume values of parameters quite different from those obtained from the BGW K-matrices but it is also necessary to introduce rather strong dependence on the density in $a_1$. We are not in a position to say whether these disagreements should be taken as an argument against the particular K-matrices used or against the K-matrix theory and BGW approximation itself.

From another point of view our work may be looked upon as a fairly successful and complete semi-empirical theory for binding energies and density distributions of nuclei.
APPENDIX

Numerical Method.

Let

\[ \xi = R \xi \quad (A.1) \]

Then

\[ \frac{d^2 \xi}{dR^2} = R \frac{d}{dR} \left( \alpha \frac{y^{2/3}}{2} + \beta \frac{y^{5/3}}{5} - y \frac{dy}{dy} + p + v c \right) = F(R, y) \quad (A.2) \]

say, since \( \xi \) is assumed to be a known function of \( y \). Also

\[ \frac{d^2}{dR^2} (R v c) = -Q R y \quad (A.3) \]

The equations were solved numerically by a generalization of the Fox-Goodwin method, which has the merit that if the successive points \( n - 1, n, n + 1 \) of integration are separated by an increment \( h \) in \( R \), the error is of order \( h^6/720 \).

Define

\[ \eta = \xi - \frac{h^2}{12} F(R, y) \quad (A.4) \]

\[ \xi = R v c + \frac{h^2}{12} Q R y \quad (A.5) \]

then it is easily shown that

\[ \eta_{n+1} = 2 \eta_n + \frac{h^2}{12} F(R_n, y_n) - \eta_{n-1} + O(h^6/720), \quad (A.6) \]

\[ \xi_{n+1} = 2 \xi_n - \frac{h^2}{12} Q R_n y_n - \xi_{n-1} + O(h^6/720) \quad (A.7) \]
and by the definitions (A.4) and (A.5)

\[ z = \frac{\xi}{R} = \left( \eta + h^2 F(R, \xi) / 12 \right) / R, \]  
(A.8)

\[ y = y(\xi), \]  
(A.9)

\[ R V_c = \xi - \frac{h^2}{12} Q \xi^2 / 12. \]  
(A.10)

Supposing \( \xi, \eta, y, z, V_c \) known at points \( n - 1 \) and \( n \), then (A.6) and (A.7) determine \( \eta_{n+1} \) and \( z_{n+1} \) to order \( h^6 \) and \( h^5 \); \( \gamma_{n+1}, V_{c_{n+1}} \) are then determined to order \( h^5 \) after one iteration of (A.8), (A.9) and (A.10).

The numerical integrations start from \( R = 0 \) with boundary conditions

\[ y = y_0, \quad V_c = V_{c_0}, \quad \frac{d y}{d R} = 0, \quad \frac{d V_c}{d R} = 0, \]

and the values at \( R = h \) were determined to order \( h^4 \) from the power series solution of (A.1) and (A.2)

\[ y = y_0 - C y_0 R^2 + C D R^4 \ldots, \]

\[ V_c = V_{c_0} - \frac{1}{6} C y_0 R^2 + \frac{1}{20} C \frac{1}{2} Q y_0 c R^4 \ldots. \]

In the special case

\[ \left( \frac{d z}{d y} \right)^2 = \frac{u^2}{1 + s \xi}, \]

\[ z = 2 u y / \left\{ (1 + s \xi) \right\}^{1/2} / 12, \]

\[ y = \frac{z}{h} \left\{ 1 + \frac{s z}{4 h} \right\}^2, \]
which with adjustable parameters u and s is sufficiently
general and was chosen for convenience, the explicit forms
of C and D are

\[ C \gamma_0 = \left( \gamma \gamma_0 - \gamma \gamma_0^2 + \beta \gamma_0^5 - P - V_{co} \right) \left( 1 + \gamma_0 \right) / 6u^2, \]

\[ D = \left( \gamma \gamma_0 - \frac{2}{3} \gamma \gamma_0^2 - \frac{5}{3} \gamma \gamma_0^5 - Q \gamma_0 / 6C \right) \left( 1 + P \gamma_0 \right) 20u^2 + 6.1 C \gamma_0^5 \left( 1 + 5\gamma_0 \right). \]

Eqs. (A.1) and (A.3) show that the solution for \( y \) depends
only on \( P + V_c \) and therefore only on the combination \( P + V_{co} \) of input parameters. For the potential \( V_c \) there is,
however, a boundary condition

\[ V_c = \frac{Q A}{R} \]

at the outside of the nucleus, which was satisfied at the
end of each integration by making a transformation

\[ P \rightarrow P - \delta, \]

\[ V_c \rightarrow V_c + \delta, \]

at all points. Thus the Coulomb potential and separation
energy were determined without ambiguity.
REFERENCES


E. Feenberg, Shell Theory of Nucleus, Princeton University Press.


L.I. Schiff, Phys. Rev., 84 (1951) 1.

84 (1951) 10.

86 (1952) 856.


This paper is referred to in this work as BGW.


15. N. V. Findler, Nuclear Physics, 8 (1958) 338.


17. Ayres, Hornyak, Chan and Fann, Nuclear Physics, 29 (1962) 212.


19. M. A. Naqvi, Nuclear Physics, 10 (1959) 256.


K. Kumar, K. J. Le Couter and M. K. Roy, Nuclear Physics, 42 (1963) 529.
31. Tables of Integral Transforms, Vol. 1, edited by
   Erdélyi, Magnus, Oberhettinger, and Tricomi,
   (McGraw Hill, 1954) p. 183