

INTERNUCLEON POTENTIALS AND THE  
CORRELATION PROBLEM IN NUCLEI

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## ABSTRACT

An investigation is made into the choice of internucleon potentials which are appropriate for nuclear structure calculations. Methods of constructing and calculating effective interactions are suggested and tested for simple nuclear systems. The results obtained show that good agreement with the experimental data can be achieved with effective interactions, but they also indicate that improved methods are needed for calculating realistic phenomenological potentials. The fitting of potentials to the high-energy two-nucleon data requires hard-core or velocity-dependent potentials; static soft-core potentials provide only part of the nuclear interaction. However a static potential fitted to the low-energy data gives a useful starting point for calculating nuclear interactions so a method is given by which the parameters of the neutron-proton potential may be calculated by a simultaneous solution of the equations associated with the deuteron.



## CHAPTER 1

## 1.1 Introduction

In nonrelativistic quantum mechanics the stationary states of a many-body system are obtained by solving the time-independent Schrödinger equation

$$H\underline{\psi} = E\underline{\psi} \quad (1.1)$$

subject to the boundary condition that  $\underline{\psi}$  vanishes at infinity. For a system containing  $A$  particles the Hamiltonian  $H$  is given by

$$H = \sum_{i=1}^A \frac{-\hbar^2}{2m_i} \nabla_i^2 + V \quad (1.2)$$

consisting of a kinetic energy term, expressed as a sum of single-particle energies, and a potential energy operator  $V$ . If  $V$  is also expressible as a sum of single-particle operators

$$V = \sum_{i=1}^A V_i \quad (1.3)$$

the Schrödinger equation can be solved since it is separable as a system of  $A$  independent single-particle equations, and the corresponding solution  $\underline{\psi}_0$  is a suitably symmetrized product of single-particle functions. In general however

$$V = \sum_{i=1}^A V_i + \sum_{i<j=2}^A V_{ij} + \sum_{i<j<k=3}^A V_{ijk} + \dots + V_{ijk\dots A} \quad (1.4)$$

When interactions involving two or more particles are present the Schrödinger equation is nonseparable in the single-particle coordinates and exact methods cannot be applied. If the interactions are weak compared with the single-particle potential energy terms, the true wavefunction  $\underline{\psi}$  will not differ greatly from the independent-particle



wavefunction  $\underline{\psi}_0$  and a good approximation to  $\underline{\psi}$  may be obtained from  $\underline{\psi}_0$  by perturbation theory.

If we assume that  $\underline{\psi}$ , like  $\underline{\psi}_0$ , can be simply expressed as a suitably symmetrized product of single-particle functions, we have the self-consistent field approximation [1] in which the particle motions are considered separately and the effects of the interactions accounted for by an average field. Since the particle motion and the calculated field are interdependent the approximate wavefunction is determined by iteration. For a system of fermions the wavefunction is required to be antisymmetric. In its simplest form, the Hartree-Fock method approximates the wavefunction with a single configuration

$$\underline{\psi}(\vec{r}_1, \vec{r}_2 \dots \vec{r}_A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \psi_\alpha(\vec{r}_1) & \psi_\alpha(\vec{r}_2) \dots \psi_\alpha(\vec{r}_A) \\ \psi_\beta(\vec{r}_1) & \psi_\beta(\vec{r}_2) \dots \psi_\beta(\vec{r}_A) \\ \vdots & \vdots \dots \vdots \\ \psi_\nu(\vec{r}_1) & \psi_\nu(\vec{r}_2) \dots \psi_\nu(\vec{r}_A) \end{vmatrix} \quad (1.5)$$

With the trial wavefunction (1.5) minimizing the energy expectation value with respect to independent variations in the single particle functions  $\psi_\lambda$  ( $\lambda=\alpha, \beta, \dots, \nu$ ) and their complex conjugates  $\psi_\lambda^*$  gives the effective single-particle Hamiltonian

$$h_{\text{HF}}(1) = \frac{-\hbar^2}{2m_1} \nabla_1^2 + v_1 + \sum_{\mu=\alpha, \beta, \dots, \nu} \int d\vec{r}_2 \psi_\mu^*(\vec{r}_2) v_{12} \sum (-1)^{P_{(12)}} \psi_\mu(\vec{r}_2) \\ + \frac{1}{2!} \sum_{\mu, \rho=\alpha, \beta, \dots, \nu} \int d\vec{r}_2 d\vec{r}_3 \psi_\mu^*(\vec{r}_2) \psi_\rho^*(\vec{r}_3) v_{123} \sum (-1)^{P_{(123)}} \psi_\mu(\vec{r}_2) \psi_\rho(\vec{r}_3) + \dots \quad (1.6)$$

where  $P_{(12\dots n)}$  are n-particle permutation operators and p their parities.

Effective Hamiltonians such as that given in (1.6) cannot fully account for the interactions since these cannot in general be described by smooth fields. The difference between the Hartree-Fock field and the actual interaction is referred to as the residual interaction. The developments in many-body theory have attempted to account for this by using trial wavefunctions of greater complexity and by introducing effective interactions which can compensate for the crudeness of the wavefunction approximation.

More flexible trial wavefunctions are obtained by taking several configurations as in the multiconfigurational Hartree-Fock and superposition of configurations methods. If a sufficiently large number of configurations is used accurate wavefunctions may be obtained by these methods, and an exact SCF theory has been given by Löwdin [2], taking a complete set of configurations. Since the complete set contains an infinite number of configurations including not only discrete states but also continuum states, the exact theory cannot be solved. Löwdin's formulation of the theory does however relate the various methods which have been applied to many-body problems. In particular, approximating the wave operator defined by Löwdin in [3] by a function depending on interparticle distances leads to the correlation function approach.

The correlation function was introduced for helium-like atoms by Hylleraas [4] who showed that explicit dependence of the trial wavefunction on the interelectron distance resulted in more rapid convergence than could be obtained by including additional configurations. A product form

$$\prod_{i < j=2}^A f(r_{ij}) \quad (1.7)$$

was used by Jastrow [5] for calculations involving strong interactions but the resulting cluster expansion of the energy expectation value must be truncated as the increasing dimensions of the integrals make them difficult to evaluate. Using the truncated expansion the correlation function cannot be determined variationally as the neglect of the higher-order terms can lead to unboundedness of the energy expectation value [6]. Combining the product form of the correlation function with a single configuration replaces the Schrödinger Hamiltonian with an effective Hamiltonian  $HC$  where  $C$  is given by (1.7).

Using the same approximation for the wavefunction, Boys and Handy [7] have developed a method which avoids the cluster expansion by defining a transcorrelated Hamiltonian related to the Schrödinger one by a similarity transformation,

$$H_{BH} = C^{-1} H C$$

When  $H$  contains only one - and two - particle operators, use of the transcorrelated Hamiltonian requires that integrals of up to nine dimensions be evaluated, but here also the variational principle cannot be applied because of the nonhermiticity of  $H_{BH}$ .

Since the correlation function may be associated with either the wavefunction or the Hamiltonian, the introduction of a correlation function leads to effective interactions. A more rigorous formulation for determining effective interactions has been derived by Brueckner [8] and Goldstone [9]. The Brueckner formalism takes into account all two-particle correlations by replacing the interaction for two free particles with an effective interaction evaluated within the many-body

system. In the limit that the number of particles becomes very large the effective Hamiltonian in Brueckner's theory is related to the original one by a unitary transformation [8]

$$H_B = \lim_{A \rightarrow \infty} F^+ H F = F^{-1} H F$$

where  $F$  is a function depending non-locally on the particle coordinates. This method has been used successfully for calculating the properties of infinitely large systems [10], but considerable difficulty has been experienced in applying it to finite systems [11]. Numerous other methods for generating effective interactions by unitary transformations have been suggested [12] and these will be considered further in the next chapter.

## 1.2 The nuclear independent particle model

So far we have considered many-body systems in general; in this section we consider the problems which are peculiar to systems of nucleons. The SCF approximation reduces the problem of a system of interacting particles to one of non-interacting particles in a field. Although this approximation has long been applied to atomic systems its validity for describing nuclear systems has been accepted comparatively recently. In an atom the electrons move mainly in the central potential due to the nucleus and, provided their motion is only slightly perturbed by interelectronic repulsion, an independent particle model is justified. No such central potential exists to bind a nucleus; instead the binding is due to the overall effect of the internucleon forces which obviously cannot be neglected or considered as weak perturbations. Although the nuclear interactions may be strong, the motion of a nucleon need not be strongly affected by its neighbours because the exclusion principle prevents it from being scattered in to an already-occupied state [13]. Through its tendency to confine each nucleon to a particular state, the exclusion principle has the effect of smoothing-out the nucleon motion and hence the overall potential within the nucleus. In this way the nuclear independent particle model can be theoretically justified. Since the single-particle energy levels give rise to a shell structure in nuclei, there is also considerable experimental evidence to support this model [14].

In practical calculations the potential energy operator in the Hamiltonian is restricted to interactions involving no more than two particles. The reason for this restriction is that little is known

about the origin of three-(or more)-particle interactions and whether or not they contribute significantly to the properties of many-particle systems. Even if three-particle terms were present, it would be difficult to distinguish between intrinsic three-particle terms, which must be included in  $V$ , and effective three - particle terms due to pair interactions within three-particle clusters. Even with this restriction, the nuclear Hamiltonian

$$H = \frac{-\hbar^2}{2m} \sum_{i=1}^A \nabla_i^2 + \sum_{i<j=2}^A v_{ij} \quad (1.8)$$

cannot be given exactly since the two-nucleon interaction is not known. If we assume the interaction  $v_{ij}$  to be the same as that for two isolated nucleons, it can in principle be determined by fitting the two-particle Hamiltonian

$$h_{12} = \frac{-\hbar^2}{2m_1} \nabla_1^2 - \frac{-\hbar^2}{2m_2} \nabla_2^2 + v_{12} \quad (1.9)$$

to the experimental two-nucleon data. Assuming that the two-nucleon interaction may be represented by a potential, its dependence on the spin, i-spin and the internucleon distance is restricted by certain invariance conditions [5], but even after all these have been satisfied a wide range of allowable potentials remains. In particular the functional dependence of the potential on the internucleon distance is not known. By parametrizing arbitrary functional forms and fitting the parameters to the two-nucleon data, phenomenological potentials have been calculated [16].

Fitting the potentials to the high-energy ( $\geq 100$  Mev) data leads to complicated potentials containing either infinitely repulsive hard cores [17] or velocity-dependent terms [18]. Hard-core potentials cannot be used in SCF calculations as they would lead to infinite matrix

elements. The introduction of velocity-dependent terms also causes a problem in that they are not uniquely determined by the bound state energy and phase shifts of the two-nucleon system [19].

Because of these difficulties, which arise from attempting to fit the potential to all the two-body data, other potentials have been calculated which give the phase shifts only approximately but which have been adjusted to give the correct energies for light nuclei [20]. Such potentials are phenomenological effective interactions which may not be applicable to nuclei other than those to which they have been fitted. Since the solution of a system with more than two particles cannot be carried out exactly, such potentials will also depend on the approximation made for the nuclear wavefunction.

### 1.3 Outline of thesis

In the next chapter we will consider a realistic interaction and transform it to an effective interaction which may be used in calculations on nuclear systems. The transformation, which is unitary, leads to a single-parameter class of velocity-dependent potentials which are indistinguishable by the two-nucleon data. In applying the effective two-nucleon interaction to larger systems, the many-body terms induced by the transformation are neglected so the transformation parameter cannot be determined variationally [49]; a method for calculating this parameter is suggested in Section 2.2. In Chapter 3 we apply the method to nuclear matter using the Gammel, Christian and Thaler hard-core potential as the realistic interaction.

Using the same hard-core potential, the theory is developed in Chapter 4 for finite nuclei. The effective two-nucleon interaction obtained differs from those previously used in that it depends on the number of nucleons in the system. This modification is made to establish a closer relationship with the correlated wavefunction approach, and results for  $\text{He}^4$  are given showing a significant improvement in the calculated binding energy.

In Chapter 4 we take a soft-core potential fitted to the energies of light nuclei and give a more accurate method for determining the radial parts of the trial wavefunction. To fit a potential in this manner, it is important to calculate the wavefunction as accurately as possible and so we replace the approximate expression of the radial functions as harmonic oscillator functions with a direct numerical solution of the Hartree-Fock equations by finite differences. The resulting energy



for the helium nucleus is compared with values obtained using correlated wavefunctions.

The finite difference method is used in Chapter 6 to calculate neutron-proton potentials satisfying the low-energy two-nucleon data. Previous methods have involved the iterative solution of only some of the potential parameters and a systematic determination of the remaining parameters [21]. Here it is possible to solve the coupled differential equations of the S-and D-radial functions of the deuteron simultaneously with the integral equations for the percentage D-state and quadrupole moment of the deuteron, and the triplet effective range for low-energy neutron-proton scattering. Since this gives only the triplet neutron-proton potential, the calculated potential is insufficient for a calculation of the binding energy of a nucleus such as  $\text{He}^4$  since this would require in addition a knowledge of the neutron-neutron and proton-proton potentials and possibly different potentials for singlet states.

## CHAPTER 2

## 2.1 Method of unitary transformations

From the work of Baker, Green, Moskowski and others [18], it is known that the effects due to an infinitely repulsive core in the two-nucleon problem can be reproduced by repulsive velocity-dependent potentials. Since reasonable fits to the two-nucleon data have been obtained with hard-core static potentials, it is not necessary to postulate forms for the velocity-dependent potentials and fit these to the data. Instead velocity-dependent potentials can be derived from static ones by the method of unitary transformations which leaves the energy of the deuteron bound state and the scattering matrix unchanged and so, in this sense, generates equivalent interactions [22].

The two-nucleon Schrödinger equation

$$\left[ \frac{\vec{p}_1^2}{2m_1} + \frac{\vec{p}_2^2}{2m_2} + v(\vec{r}_1 - \vec{r}_2) \right] \psi = E\psi \quad (2.1)$$

is separable in terms of relative and centre of mass coordinates

$$\vec{r} = \vec{r}_1 - \vec{r}_2 \quad ; \quad \vec{R} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}$$

with corresponding momenta

$$\vec{p} = \frac{m_2 \vec{p}_1 - m_1 \vec{p}_2}{m_1 + m_2} \quad ; \quad \vec{P} = \vec{p}_1 + \vec{p}_2$$

We are concerned only with the equation in the relative coordinates

$$(m = \frac{m_1 m_2}{m_1 + m_2})$$

$$\left[ \frac{\vec{p}^2}{2m} + v(r) \right] \phi(\vec{r}) = \epsilon \phi(\vec{r}) \quad (2.2)$$

From considerations of permutation symmetry the possible two-nucleon states may be classified according to the following table

TABLE 1

State	S	T	$\ell$	$P_\alpha$
triplet odd $\alpha=1$	1	1	odd	$\frac{1}{16}(3+\vec{\tau}_1 \cdot \vec{\tau}_2)(3+\vec{\sigma}_1 \cdot \vec{\sigma}_2)$
triplet even $\alpha=2$	1	0	even	$\frac{1}{16}(1-\vec{\tau}_1 \cdot \vec{\tau}_2)(3+\vec{\sigma}_1 \cdot \vec{\sigma}_2)$
singlet even $\alpha=3$	0	1	even	$\frac{1}{16}(3+\vec{\tau}_1 \cdot \vec{\tau}_2)(1-\vec{\sigma}_1 \cdot \vec{\sigma}_2)$
singlet odd $\alpha=4$	0	0	odd	$\frac{1}{16}(1-\vec{\tau}_1 \cdot \vec{\tau}_2)(1-\vec{\sigma}_1 \cdot \vec{\sigma}_2)$

in which S is the total spin, T the total i-spin,  $\ell$  the relative orbital angular momentum and P the corresponding projection operator. In general the static potential  $v(r)$  will contain both central and tensor parts for which the radial dependences may be different for different states i.e.

$$v(r) = \sum_{\alpha} (v_{\alpha}^c(r) + v_{\alpha}^t(r)S_{12})P_{\alpha} \quad (2.3)$$

where  $S_{12}$  is the tensor operator :

$$S_{12} = \frac{3}{r^2} (\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \quad (2.4)$$

Since  $\sum_{\alpha} P_{\alpha} = 1$ , the relative Hamiltonian can be expressed as

$$h = \frac{p^2}{2m} + v(r) = \sum_{\alpha} h_{\alpha} P_{\alpha} \quad (2.5a)$$

where

$$h_{\alpha} = \frac{p^2}{2m} + v_{\alpha}^c(r) + v_{\alpha}^t(r)S_{12} \quad (2.5b)$$

The most general unitary transformation operator which does not mix the charge-spin states of the two-nucleon system has been given by Rohl and Stocker [23]:

$$U = e^{i \sum_{\alpha} \Omega_{\alpha} P_{\alpha}}$$

where the  $\Omega_{\alpha}$  are hermitian. Since  $P_{\alpha} P_{\beta} = \delta_{\alpha\beta}$  the  $\Omega_{\alpha} P_{\alpha}$  commute with one another and so  $U$  can be factored as

$$U = \prod_{\alpha} u_{\alpha} = \prod_{\alpha} e^{i \Omega_{\alpha} P_{\alpha}}$$

Applying the unitary transformation to the Hamiltonian given in (2.5) we obtain

$$\begin{aligned} \tilde{h} &= \prod_{\alpha} u_{\alpha} \left( \sum_{\beta} h_{\beta} \right) \prod_{\gamma} u_{\gamma}^{\dagger} \\ &= \sum_{\beta} \left[ \prod_{\alpha \neq \beta} u_{\alpha} \left( u_{\beta} h_{\beta} u_{\beta}^{\dagger} \right) \prod_{\gamma \neq \beta} u_{\gamma}^{\dagger} \right] \end{aligned}$$

Each factor and hence the product of  $u_{\alpha}$ 's ( $\alpha \neq \beta$ ) commutes with  $u_{\beta} h_{\beta} u_{\beta}^{\dagger}$  for all  $\beta$  so

$$\begin{aligned} \tilde{h} &= \sum_{\beta} u_{\beta} h_{\beta} u_{\beta}^{\dagger} \\ &= \sum_{\beta} e^{i \Omega_{\beta} P_{\beta}} h_{\beta} e^{-i \Omega_{\beta} P_{\beta}} \end{aligned}$$

Expanding each term of  $\tilde{h}$  as

$$e^{i \Omega_{\beta} P_{\beta}} h_{\beta} e^{-i \Omega_{\beta} P_{\beta}} = h_{\beta} + i [\Omega_{\beta} P_{\beta}, h_{\beta}] + \frac{i^2}{2!} [\Omega_{\beta} P_{\beta}, [\Omega_{\beta} P_{\beta}, h_{\beta}]] + \dots$$

the first commutator simplifies to

$$[\Omega_{\beta} P_{\beta}, h_{\beta}] = [\Omega_{\beta}, h_{\beta}] P_{\beta}$$

since  $[P_{\beta}, h_{\beta}] = 0$ . Similarly for the second commutator :

$$\begin{aligned}
[\Omega_\beta P_\beta, [\Omega_\beta P_\beta, h_\beta]] &= [\Omega_\beta, [\Omega_\beta, h_\beta]] P_\beta^2 \\
&= [\Omega_\beta, [\Omega_\beta, h_\beta]] P_\beta
\end{aligned}$$

and so on for the higher-order terms. Hence

$$\tilde{h} = \sum_{\beta} \tilde{h}_{\beta} P_{\beta} \quad (2.6a)$$

where

$$\tilde{h}_{\beta} = e^{i\Omega_{\beta} h_{\beta}} e^{-i\Omega_{\beta}} \quad (2.6b)$$

Thus the different state-dependent parts of the Hamiltonian may be transformed independently. Conditions on the hermitian operators  $\Omega_{\alpha}$  have been given by Middelstaedt and Ristig [24] to ensure the conservation of phase shifts.

These conditions can be easily expressed if we restrict our consideration to a class of unitary transformations which affect only the magnitude of the relative coordinate :

$$r \rightarrow UrU^{\dagger} \equiv \tilde{r} \quad (2.7)$$

Following the method of Bell [25], which used the norm-conserving property of unitary transformations, Ristig and Kistler [26] have given the form of the transformed Hamiltonian and the relative wavefunction for state-independent transformations. Since there is no overlap between the different charge-spin states this can be generalized to state-dependent transformations.

$$r \rightarrow \tilde{r}_{\alpha} \quad \text{in each } h_{\alpha} \quad (2.8)$$

and gives an expression for the transformed Hamiltonian in terms of the Jacobians  $G_{\alpha}$  of the radial transformations

$$\tilde{h} = \sum_{\alpha} \left[ G_{\alpha}^{-\frac{1}{2}} (h_{\alpha})_{r \rightarrow \tilde{r}_{\alpha}} G_{\alpha}^{\frac{1}{2}} \right] \quad (2.9)$$

in which

$$G_{\alpha}^{-\frac{1}{2}} = \frac{\tilde{r}_{\alpha}}{r} \sqrt{\frac{\partial \tilde{r}_{\alpha}}{\partial r}} \quad (2.10)$$

and  $(h_{\alpha})_{r \rightarrow \tilde{r}_{\alpha}}$  means that  $r$  is replaced by  $\tilde{r}_{\alpha}$  in  $h_{\alpha}$ . The condition that the transformation preserve the phase shifts can now be applied directly to the transformed radial variaties  $\tilde{r}_{\alpha}$  viz

$$\tilde{r}_{\alpha} \underset{r \rightarrow \infty}{=} r + O\left(\frac{1}{r}\right) \quad (2.11)$$

The transformed Hamiltonian can be deduced from (2.9). Since  $G_{\alpha}$  commutes with the terms of the static potential

$$v^c(r) + v^t(r) S_{12} \rightarrow v^c(\tilde{r}) + v^t(\tilde{r}) S_{12}$$

where the subscript  $\alpha$  has been omitted since the general form is the same for all states. The kinetic energy operator is most easily transformed by re-expressing it as

$$t = \frac{1}{2m} \left( p_r^2 + \frac{\ell^2}{r^2} \right) \quad (2.12)$$

where  $p_r$  is the radial momentum operator

$$p_r = \frac{\hbar}{i} \frac{1}{r} \frac{\partial}{\partial r} r = \frac{1}{2} \left( \frac{\vec{r} \cdot \vec{p}}{r} + \frac{\vec{p} \cdot \vec{r}}{r} \right)$$

and  $\vec{\ell} = \vec{r} \times \vec{p}$  the angular momentum operator.  $G_{\alpha}$  commutes with  $\vec{\ell}$  so

$$\tilde{t} = \frac{1}{2m} \left\{ \frac{1}{G_{\alpha}^2} (p_r)_{r \rightarrow \tilde{r}}^2 G_{\alpha}^{\frac{1}{2}} + \frac{\ell^2}{\tilde{r}^2} \right\}$$

The transformed radial momentum  $\tilde{p}_r$  is

$$\tilde{p}_r = G_{\alpha}^{-\frac{1}{2}} \left( \frac{\hbar}{i} \frac{1}{\tilde{r}} \frac{\partial}{\partial \tilde{r}} \tilde{r} \right) G_{\alpha}^{\frac{1}{2}}$$

which, with  $G^{-\frac{1}{2}} = \frac{\tilde{r}}{r} \sqrt{\frac{\partial \tilde{r}}{\partial r}}$ , becomes

$$\tilde{p}_r = B^{\frac{1}{2}} p_r B^{\frac{1}{2}}$$

where  $B^{-1} = \frac{\partial \tilde{r}}{\partial r}$ . Since  $G^{-\frac{1}{2}} (p_r)_{r \rightarrow \tilde{r}} G^{\frac{1}{2}} = \left[ G^{-\frac{1}{2}} (p_r)_{r \rightarrow \tilde{r}} G^{\frac{1}{2}} \right]^2$  we get

$$h = \frac{1}{2m} [B^{\frac{1}{2}} p_r B^{\frac{1}{2}}]^2 + v^c(\tilde{r}) + v^t(\tilde{r}) S_{12} \quad (2.13)$$

If  $B^{\frac{1}{2}}$  is a function which can be expanded as a power series in  $r$ , use can be made of the commutation relation

$$[p_r, B^{\frac{1}{2}}] = \frac{\hbar}{2i} B^{-\frac{1}{2}} \frac{\partial B}{\partial r}$$

to derive alternative expressions for  $\tilde{p}_r^2$  :

$$\begin{aligned} \tilde{p}_r^2 &= B^2 p_r^2 + \frac{2\hbar}{i} B \frac{\partial B}{\partial r} - \frac{\hbar^2}{2} B \frac{\partial^2 B}{\partial r^2} - \frac{\hbar^2}{4} \left( \frac{\partial B}{\partial r} \right)^2 \\ &= B p_r^2 B + \frac{\hbar^2}{2} B \frac{\partial^2 B}{\partial r^2} - \frac{\hbar^2}{4} \left( \frac{\partial B}{\partial r} \right)^2 \\ &= \frac{1}{2} (B^2 p_r^2 + p_r^2 B^2) + \frac{\hbar^2}{2} B \frac{\partial^2 B}{\partial r^2} + \frac{3\hbar^2}{4} \left( \frac{\partial B}{\partial r} \right)^2 \end{aligned}$$

Using the last of these gives the velocity-dependent potential  $w$

$$\begin{aligned} w &= \frac{1}{2m} \left[ \frac{1}{2} \left\{ (B^2 - 1) p_r^2 + p_r^2 (B^2 - 1) \right\} + \ell^2 \left( \frac{1}{\tilde{r}^2} - \frac{1}{r^2} \right) + \frac{\hbar^2}{2} B \frac{\partial^2 B}{\partial r^2} + \frac{3\hbar^2}{4} \left( \frac{\partial B}{\partial r} \right)^2 \right] \\ &+ v^c(\tilde{r}) + v^t(\tilde{r}) S_{12} \quad (2.14) \end{aligned}$$

and

$$\tilde{h} = t + w \quad \text{in the state-independent case}$$

and

$$\tilde{h} = t + \sum_{\alpha} w_{\alpha} \quad \text{in the state-dependent case.}$$

From (2.14) it can be seen that the hard cores of the static potentials

are removed if

$$\tilde{r} = r_c \text{ at } r = 0.$$

The method of unitary transformations described so far applies only to two-particle systems. Although the velocity-dependent potentials generated are equivalent in the sense that they give the same deuteron binding energy and nucleon-nucleon scattering phase shifts, their use in many-nucleon systems will lead to different properties [27] so the next problem to be considered is the selection of the appropriate potential for a given system.



## 2.2 Determination of the effective velocity-dependent potential

The extension of the method of unitary transformations to many particle systems ( $A \geq 3$ ) may be carried out by

either (i) applying a unitary transformation with an operator  $U = e^{i\Omega_{123\dots A}}$ , where  $\Omega$  is hermitian, so that the reduction to the two-particle problem gives the results obtained in the previous section or (ii) regarding the velocity-dependent potential obtained after the two-nucleon transformation as an effective two-nucleon interaction which is no less realistic than the original static one.

By taking

$$U = e^{i \sum_{j < k = 2}^A \Omega_{jk}}$$

induced many-body forces appear in the effective Hamiltonian unless the approximation

$$e^{i \sum_{j < k = 2}^A \Omega_{jk}} \approx 1 + i \sum_{j < k = 2}^A \Omega_{jk} \quad (2.15)$$

is made, in which case only operators involving up to three particles occur [28]. Since the three-particle (and higher-order if the approximation (2.15) is not used) terms are difficult to evaluate and interpret, they are generally neglected, and the approaches (i) and (ii) then lead to the same formulation of the problem. Thus we use the approximation

$$H_{\text{eff}} = \sum_i \frac{p_i^2}{2m_i} + \sum_{i < j = 2}^A w_{ij} \approx U^\dagger H U \quad (2.16)$$

where

$$H = \sum_i \frac{p_i^2}{2m_i} + \sum_{i < j = 2}^A v_{ij}$$

We now restrict the transformations so that the effective Hamiltonian is obtained by a one-parameter class of radial transformations which, for simplicity in the following discussion, we take to be state-independent:

$$r_{ij} \rightarrow \tilde{r}_{ij} = f(\beta, r_{ij}) \quad (2.17a)$$

where  $\beta$  is the transformation parameter, and

$$f(\beta, 0) = r_c, \quad \text{the hard core radius } \geq 0 \quad (2.17b)$$

$$\text{and} \quad f(\beta, r) \underset{r \rightarrow \infty}{=} r + O\left(\frac{1}{r}\right) \quad (2.17c)$$

to conserve the phase shifts.

Up to this point we have discussed in detail only the two-nucleon case for which the effective velocity-dependent potential has been defined in (2.16). This is the potential used by other authors previously and which we will use in the nuclear matter calculations. When the number of nucleons is finite, an alternative extension of the results of the preceding section to many-nucleon systems is possible, and this will also be considered when we calculate the energies of light nuclei. Since the remainder of this section is not affected by the exact form of  $w_{ij}$ , we leave the development of the effective interaction for finite nuclei until later. For either form we may write

$$H_{\text{eff}} = T + V(\beta)$$

where  $T$  is the total kinetic energy operator and  $V$  the potential energy operator depending on the transformation parameter  $\beta$ .

The Schrödinger equation to be solved is now

$$H_{\text{eff}} \underline{\psi} = [T + V(\beta)] \underline{\psi} = E \underline{\psi} \quad (2.18)$$

It has been shown by Löwdin [29] that satisfaction of the virial theorem is a necessary but not sufficient condition for a trial wavefunction to be an accurate solution of the Schrödinger equation. In general, variationally determined wavefunctions do not satisfy the virial theorem. In the special case that the variational parameter is a scale factor which uniformly distorts the position vectors of all the particles, it is found that the scaled wavefunction is an improvement over the unscaled one because the virial theorem is satisfied. The results obtained by Löwdin could also have been obtained by introducing the inverse scale factor in the kinetic and potential energy operators, leaving the relation between the kinetic and potential energy expectation values unchanged. Although the derivation given by Löwdin follows an earlier one due to Fock [30] in that the potential function is assumed to be a homogeneous function of the coordinates, this is not a necessary restriction and a generalization has been given by Epstein and Hirschfelder [31].

The limitation on the usefulness of the virial theorem is that it can only be used to determine one parameter, whereas the variational principle provides as many equations as there are variational parameters. Except in the case of the scale factor the virial theorem and the variational principle do not coincide so, in general, the virial theorem provides an independent test of the degree to which a trial wavefunction approximates an eigenfunction of the Hamiltonian.

The result in which we are principally interested is the relationship between the kinetic energy expectation value and the expectation value of a term involving the potential energy operator. This relationship has been used to calculate solutions of molecular problems by Slater [32] who noted that when the total energy is stationary with respect to small variations in the wavefunction, the relation between the kinetic and potential energies changes much more rapidly since the total energy is calculated as the comparatively small difference of two larger terms. Since the transformation parameter  $\beta$  occurs only in the potential energy operator  $V$ , the relationship between the kinetic and potential energy operators demanded by the virial theorem with any given trial wavefunction can be satisfied by an appropriate choice of  $\beta$ .

Hence we will determine  $\beta$  by requiring that

$$\langle T \rangle = \frac{i}{2\hbar} \left\langle \left[ \sum_k \vec{r}_k \cdot \vec{p}_k, V(\beta) \right] \right\rangle \quad (2.19)$$

## CHAPTER 3

## 3.1 Nuclear matter

The state of nuclear matter is an approximation of the central region within a very large nucleus. It is an idealized state in that the Coulomb repulsion between protons is ignored and the numbers of protons and neutrons are taken to be equal and infinitely large so that symmetry and surface effects can also be neglected. That such a system should form a stable configuration is to be expected from the property of saturation of nuclear forces i.e. the binding energy per nucleon is approximately constant for all but the very light nuclei. The Bethe-Weizsäcker empirical mass formula expresses the binding energies of large nuclei in terms of the proton number  $Z$ , neutron number  $N$ , and their sum  $A = N + Z$ :

$$\begin{aligned} \text{B.E. (MeV)} = & - 16.11 A + (20.65 - 48.00 A^{-\frac{1}{3}}) \frac{[(N-Z)^2 + 2|N-Z|]}{A} \\ & + 20.21 A^{\frac{2}{3}} + 0.8076 A^{-\frac{1}{3}} Z^2 (1 - 0.7636 Z^{-\frac{2}{3}} - 2.29 A^{-\frac{2}{3}}) \end{aligned} \quad (3.1)$$

where we have used the empirical values given by Seeger [33]. It is the first term in (3.1) in which we are interested since this gives the volume energy per nucleon as  $- 16.11$  Mev. The remaining terms give the symmetry energy, the surface energy and the coulomb energy and these do not contribute to the energy per nucleon in nuclear matter.

Evidence from electron scattering indicates that the central density is approximately constant from nucleus to nucleus and an average nucleon density is defined through the radius of the volume per particle,  $r_0$ , by

$$\text{Number density, } \rho = \left( \frac{4\pi r_0^3}{3} \right)^{-1} \quad (3.2)$$

where  $r_0$  has been deduced from electron scattering experiments as [34]

$$r_0 \approx 1.07 \text{ fm} \quad (3.3)$$

In nuclear matter it is assumed that the number of nucleons  $A$  and the volume  $V$  which they occupy are both very large, and that as  $A$  and  $V$  become infinitely large the density  $\rho = A/V$  remains finite. Then the nucleon wavefunctions are plane waves in coordinate space and the normalized single-particle functions are

$$|n\rangle = \frac{e^{-i\vec{k}_n \cdot \vec{r}_n}}{\sqrt{V}} \chi_{m_s n} \xi_{m_t n} \quad (3.4)$$

where  $\chi$  and  $\xi$  are spin and  $i$ -spin functions.

## 3.2 Calculation of properties of nuclear matter

Using the Hamiltonian

$$H = \sum_{i=1}^A t_i + \frac{1}{2} \sum_{i \neq j=1}^A w_{ij} \quad (3.5)$$

the total energy is

$$E = \sum_{i=1}^A \langle i | t | i \rangle + \frac{1}{2} \sum_{i \neq j=1}^A [\langle ij | w | ij \rangle - \langle ij | w | ji \rangle] \quad (3.6)$$

for which the sum over the states  $i$  is given by

$$\sum_i = \sum_{\vec{k}_i} \sum_{m_{S_i}} \sum_{m_{\tau_i}}$$

Since  $A$  and  $V$  are very large the range of values of  $\vec{k}$  is almost continuous so we can make the approximation

$$\sum_{\vec{k}_i} \approx \frac{V}{(2\pi)^3} \int d\vec{k}_i \quad (3.7)$$

where  $\frac{V}{(2\pi)^3}$  is the density of wave vectors in phase space. The occupied states fill what is referred to as the Fermi Sea in which  $0 \leq |\vec{k}| \leq k_F$ , the Fermi momentum. The Fermi momentum is obtained through the relation

$$\sum_{i=1}^A 1 = \sum_{m_{S_i}} \sum_{m_{\tau_i}} \frac{V}{(2\pi)^3} \int d\vec{k}_i = A$$

from which the spin-i-spin summation gives a factor 4 and the  $\vec{k}$ -integral a factor  $\frac{4}{3} \pi k_F^3$ .

$$\text{Thus} \quad k_F^3 = \frac{3\pi^2}{2} \left( \frac{A}{V} \right) \quad (3.8)$$

and through the number density the average radius per nucleon can be related to the Fermi momentum as

$$r_0 = \left( \frac{9\pi}{8} \right)^{\frac{1}{3}} \frac{1}{k_F} \quad (3.9)$$

The total kinetic energy is

$$T = \sum_i \langle i | t | i \rangle = \frac{V}{(2\pi)^3} \sum_{m_{S_i}} \sum_{m_{T_i}} \int d\vec{k}_i \int d\vec{r} \frac{e^{i\vec{k}_i \cdot \vec{r}}}{\sqrt{V}} \frac{\hbar^2 k_i^2}{2m} \frac{e^{-i\vec{k}_i \cdot \vec{r}}}{\sqrt{V}}$$

which, after carrying out the integrations and expressing  $\frac{A}{V}$  in terms of  $k_F$  using (3.8), gives the kinetic energy per nucleon :

$$\frac{T}{A} = \frac{3}{10} \frac{\hbar^2 k_F^2}{m} \quad (3.10)$$

To calculate the matrix elements of the interaction we transform to the relative and centre of mass coordinates

$$\vec{r} = \vec{r}_1 - \vec{r}_2, \quad \vec{R} = \frac{1}{2} (\vec{r}_1 + \vec{r}_2) \quad (3.11)$$

with corresponding wave vectors

$$\vec{k} = \frac{1}{2} (\vec{k}_1 - \vec{k}_2), \quad \vec{k} = \vec{k}_1 + \vec{k}_2$$

The static potential from which our velocity dependent potential is derived is that of Gammel, Christian and Thaler [34] which has the form

$$V = \sum_{\alpha=1}^4 v_{\alpha}^c(r) P_{\alpha} + \sum_{\alpha=1}^2 v_{\alpha}^t(r) P_{\alpha} S_{12} \quad (3.12)$$

where  $\alpha$  labels the charge-spin states and  $P_{\alpha}$  are the projection operators given previously in Table 1. The radial dependences  $v_{\alpha}^c$  and  $v_{\alpha}^t$  are all taken to be Yukawa shapes for which the depths and inverse ranges are given in the following table,



Table 2

Parameters of the Gammel, Christian, Thaler potential		
	Depth (MeV)	Inverse range (fm <sup>-1</sup> )
$v_1^c$	-150.0	1.5
$v_2^c$	-6395	2.937
$v_3^c$	-905.6	1.7
$v_4^c$	113.0	1.0
$v_1^t$	57.50	1.12
$v_2^t$	- 45.00	0.734

and hard cores of radius 0.5 fm are included in each of the terms.

In nuclear matter the matrix elements of the tensor terms vanish on summing over the spins, and the spin-i-spin sums give the following factors for the direct and exchange terms of the central potential.

Table 3

$\alpha$	$\sum \langle m_{S_1} m_{T_1} m_{S_2} m_{T_2}   P_\alpha   m_{S_1} m_{T_1} m_{S_2} m_{T_2} \rangle$	$\sum \langle m_{S_1} m_{T_1} m_{S_2} m_{T_2}   P_\alpha   m_{S_2} m_{T_2} m_{S_1} m_{T_1} \rangle$
1	9	9
2	3	-3
3	3	-3
4	1	1

In Table 3 the sums are over  $m_{S_1}, m_{S_2}, m_{T_1}$  and  $m_{T_2}$ . These factors multiplying the spatial integrals of the direct and exchange integrals which are then integrated over  $\vec{k}_1$  and  $\vec{k}_2$  to obtain the contributions to the potential energy per nucleon. The limits  $|\vec{k}_1| \leq k_F$  and  $|\vec{k}_2| \leq k_F$  give the restrictions on the angular integration over the  $\vec{k}$  vector:

$$\begin{aligned} \int d\Omega_{\vec{k}} &= 4\pi && K \leq 2(k_F - k) \\ &= 4\pi \left( \frac{k_F^2 - k^2 - \frac{1}{4}K^2}{kK} \right) && 2(k_F - k) \leq K \leq 2(k_F^2 - k^2)^{\frac{1}{2}} \\ &= 0 && 2(k_F^2 - k^2)^{\frac{1}{2}} \leq K \end{aligned}$$

Since the interaction  $w$  is dependent only on the relative coordinate we can complete the  $\vec{K}$  integration immediately giving

$$\int d\vec{K} = \frac{32\pi}{3} k_F^3 \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \quad (3.13)$$

Similarly the integral over the centre-of-mass coordinate can be performed giving a factor 1 since the coordinate transformation (3.11) does not affect the normalization. Thus we are left with the direct integrals

$$\frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} e^{i\vec{k} \cdot \vec{r}} w_{\alpha} e^{-i\vec{k} \cdot \vec{r}} \quad (3.14)$$

and the exchange integrals

$$\frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} e^{i\vec{k} \cdot \vec{r}} w_{\alpha} e^{i\vec{k} \cdot \vec{r}} \quad (3.15)$$

for which  $\alpha = 1, \dots, 4$ . The matrix elements of tensor force vanish so we need consider only the effective interaction

$$w_{\alpha} = \frac{\hbar^2}{2m} \left[ \left\{ (B^2 - 1) p_r^2 + p_r^2 (B^2 - 1) \right\} + \ell^2 \left( \frac{1}{r^2} - \frac{1}{r^2} \right) + \frac{B}{2} \frac{\partial^2 B}{\partial r^2} + \frac{3}{4} \left( \frac{\partial B}{\partial r} \right)^2 \right] + v_{\alpha}^c(\vec{r}) \quad (3.16)$$

Since plane wave states are not eigenfunctions of  $\ell^2$ , the calculations are simplified by rewriting  $w_{\alpha}$  as

$$w_\alpha = \frac{\hbar^2}{2m} \left[ \left\{ (B^2 - g - 1) p_r^2 + p_r^2 (B^2 - g - 1) \right\} + \frac{1}{2} (g p^2 + p^2 g) + \frac{B}{2} \frac{\partial^2 B}{\partial r^2} + \frac{3}{4} \left( \frac{\partial B}{\partial r} \right)^2 \right] + v^c(\tilde{r}) \quad (3.17)$$

We define the functions

$$V_0^\alpha(r) \equiv \frac{B}{2} \frac{\partial^2 B}{\partial r^2} + \frac{3}{4} \left( \frac{\partial B}{\partial r} \right)^2 + v^c(\tilde{r})$$

$$V_1^\alpha(r) \equiv \frac{2}{r} (B^2 - g - 1)$$

$$V_2^\alpha(r) \equiv \frac{r}{2} V_1^\alpha(r)$$

$$V_3^\alpha(r) \equiv g = \frac{1}{\tilde{r}^2} - \frac{1}{r^2}$$

In terms of these functions the contribution from the direct integral to the binding energy per nucleon is

$$\sum_{\alpha=1}^4 c_{\text{dir}}^\alpha \left[ \frac{k_F^3}{12\pi} \int_0^\infty V_0^\alpha(r) r^2 dr + \frac{k_F^5}{120\pi} \int_0^\infty V_2^\alpha(r) r^2 dr + \frac{k_F^5}{40\pi} \int_0^\infty V_3^\alpha(r) r^2 dr \right] \quad (3.18)$$

where the  $c_{\text{dir}}^\alpha$  are the factors given in Table 3. The details of the  $k$ -integrations and the angular coordinate space integrations are given in Appendix 1A. Similarly the contribution of the exchange integral is

$$\sum_{\alpha=1}^4 c_{\text{exch}}^\alpha \left[ \frac{2k_F^3}{\pi} \int_0^\infty V_0^\alpha(r) k_0(z) r^2 dr + \frac{2k_F^4}{4\pi} \int_0^\infty V_1^\alpha(r) k_1(z) r^2 dr + \frac{2k_F^5}{\pi} \int_0^\infty V_2^\alpha(r) k_2(z) r^2 dr + \frac{2k_F^5}{\pi} \int_0^\infty V_3^\alpha(r) k_3(z) r^2 dr \right] \quad (3.19)$$

in which  $z = 2k_F r$  and further details and the definitions of the functions  $k_0, \dots, k_3$  are given in Appendix 1B.

In our calculations we will consider two radial transformations : the first is the simplest form which has the required properties as given in (2.17) :

$$\tilde{r} = r + r_c e^{-\beta r} \quad (3.20)$$

and the second, which we use for purposes of comparison, is that used by Ristig and Kistler in their nuclear matter calculations :

$$\tilde{r} = r + \beta^{-1} \ln[1 + (e^{\beta r_{c-1}})e^{-\beta r}] \quad (3.21)$$

To determine  $\beta$  by the virial theorem (2.19) for nuclear matter we need to calculate the expectation value of the commutator

$$\frac{i}{2\hbar A} [\sum_k \vec{r}_k \cdot \vec{p}_k, V(\beta)] = \frac{\langle T \rangle}{A} \quad (3.22)$$

where, as with the energy, we must work with the value per nucleon.

The commutator simplifies as

$$\begin{aligned} [\sum_k \vec{r}_k \cdot \vec{p}_k, V(\beta)] &= \frac{1}{2} \sum_k [\vec{r}_k \cdot \vec{p}_k, \sum_{i,j}^{\neq} w_{ij}] \\ &= \frac{1}{2} \sum_k \sum_{i,j}^{\neq} \left( [\vec{r}_k \cdot \vec{p}_k, w_{ij}] \delta_{ik} + [\vec{r}_k \cdot \vec{p}_k, w_{ij}] \delta_{jk} \right) \\ &= \frac{1}{2} \sum_{i,j}^{\neq} \left( [\vec{r}_i \cdot \vec{p}_i, w_{ij}] + [\vec{r}_j \cdot \vec{p}_j, w_{ij}] \right) \\ &= \frac{1}{2} \sum_{i,j}^{\neq} [(\vec{r}_i \cdot \vec{p}_i + \vec{r}_j \cdot \vec{p}_j), w_{ij}] \end{aligned}$$

After the transformation (3.11) to relative and centre of mass coordinates this becomes, for each pair of  $i, j$  values

$$\frac{1}{2} [\vec{r} \cdot \vec{p} + \vec{R} \cdot \vec{P}], w]$$

where  $\vec{p} = \hbar \vec{k}$  and  $\vec{P} = \hbar \vec{K}$  and, since the integrals are separable in these coordinates and  $w$  depends only on the relative coordinate, we need only to calculate  $\frac{1}{2} [\vec{r} \cdot \vec{p}, w]$ . For the part of  $w$  which contains a function of  $r$  multiplied by an operator commutes with  $\vec{r} \cdot \vec{p}$ , e.g.  $\ell^2$  or 1, we use the commutation relation [35]

$$[\vec{r} \cdot \vec{p}, f(r)] = \frac{\hbar}{i} r \frac{\partial f}{\partial r} \quad (3.23)$$

The remainder of  $w$  is expressed as a symmetrized product of a function  $f(r)$  and the square of the relative radial momentum for which

$$[\vec{r} \cdot \vec{p}, \frac{1}{2}(f p_r^2 + p_r^2 f)] = \frac{1}{2}(f [\vec{r} \cdot \vec{p}, p_r^2] + [\vec{r} \cdot \vec{p}, f] p_r^2 + p_r^2 [\vec{r} \cdot \vec{p}, f] + [\vec{r} \cdot \vec{p}, p_r^2] f)$$

This is evaluated using the commutation relation (3.23) and also

$$[\vec{r} \cdot \vec{p}, p_r^2] = 2i\hbar p_r^2 \quad (3.24)$$

With  $w$  of the form given in (3.16) we have the following expression

for  $[\vec{r} \cdot \vec{p}, w]$  :

$$\begin{aligned} \frac{2\hbar}{i} \int_{\alpha} \frac{1}{2m} \left[ -\frac{1}{2} \left\{ \left( B^2 - rB \frac{\partial B}{\partial r} - 1 \right) p_r^2 + p_r^2 \left( B^2 - rB \frac{\partial B}{\partial r} - 1 \right) \right\} - \ell^2 \left( \frac{r}{r^3} \frac{\partial \tilde{r}}{\partial r} - \frac{r}{r^2} \right) \right. \\ \left. + \frac{\hbar^2}{4} rB \frac{\partial^3 B}{\partial r^3} + \hbar^2 r \frac{\partial B}{\partial r} \frac{\partial^2 B}{\partial r^2} \right] + \frac{r}{2} \frac{\partial}{\partial r} v_{\alpha}^c(\tilde{r}) + \frac{r}{2} \frac{\partial}{\partial r} v_{\alpha}^t(\tilde{r}) S_{12} \quad (3.25) \end{aligned}$$

The general form of this expression is the same as that for  $w$  and so we use the same procedures to calculate the two-particle matrix elements.

### 3.3 Results and conclusions

Using the Gammel-Christian-Thaler potential and the transformation (3.20) the binding energy per nucleon is calculated with the Fermi momentum  $k_F$  as a variational parameter. Typical BE/A curves are shown in Figure 1.

If  $\beta$  is determined variationally, the optimum value  $\beta_{\text{var}}$  is  $1.2 \text{ fm}^{-1}$  and the corresponding binding energy per nucleon  $-17.97 \text{ MeV}$  at  $k_F = 2.0 \text{ fm}^{-1}$ . The empirical value of the average radius per nucleon  $r_0 = 1.07 \text{ fm}$  corresponds to a value for  $k_F$  of  $1.42 \text{ fm}^{-1}$  so these values are both too large. The energy value is particularly bad since the Hartree-Fock approximation used here does not include the binding due to the tensor force which has been estimated by Brueckner [36] to be approximately  $6 \text{ MeV}$  per nucleon.

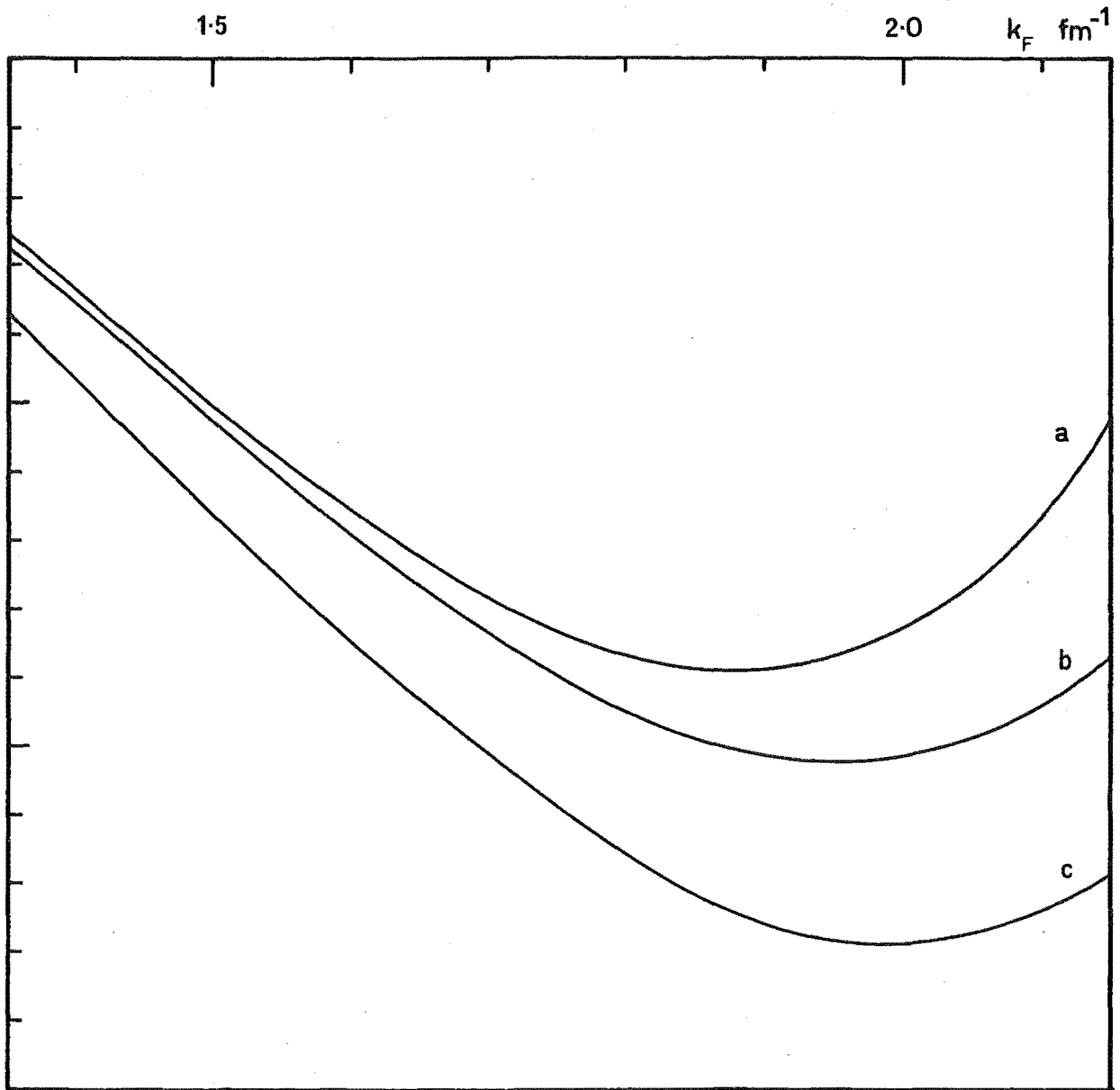
By adjusting  $\beta$  so that the virial theorem is satisfied when the energy is a minimum with respect to variations in  $k_F$ , we obtain the value  $\beta_{\text{vir}} = 1.35 \text{ fm}^{-1}$  with

$$\text{BE/A} = -12.47 \text{ MeV}$$

$$k_F = 1.89 \text{ fm}^{-1}$$

The energy value obtained here compares favourably with the  $-12.5 \text{ MeV}$  obtained by Brueckner [36] using the Gammel-Christian-Thaler potential without tensor forces. The parameter  $r_0$  obtained in the present calculation is  $0.80 \text{ fm}$ , giving a density slightly higher than that obtained by the Brueckner method which gives  $r_0 = 0.95 \text{ fm}$ .

FIGURE 1



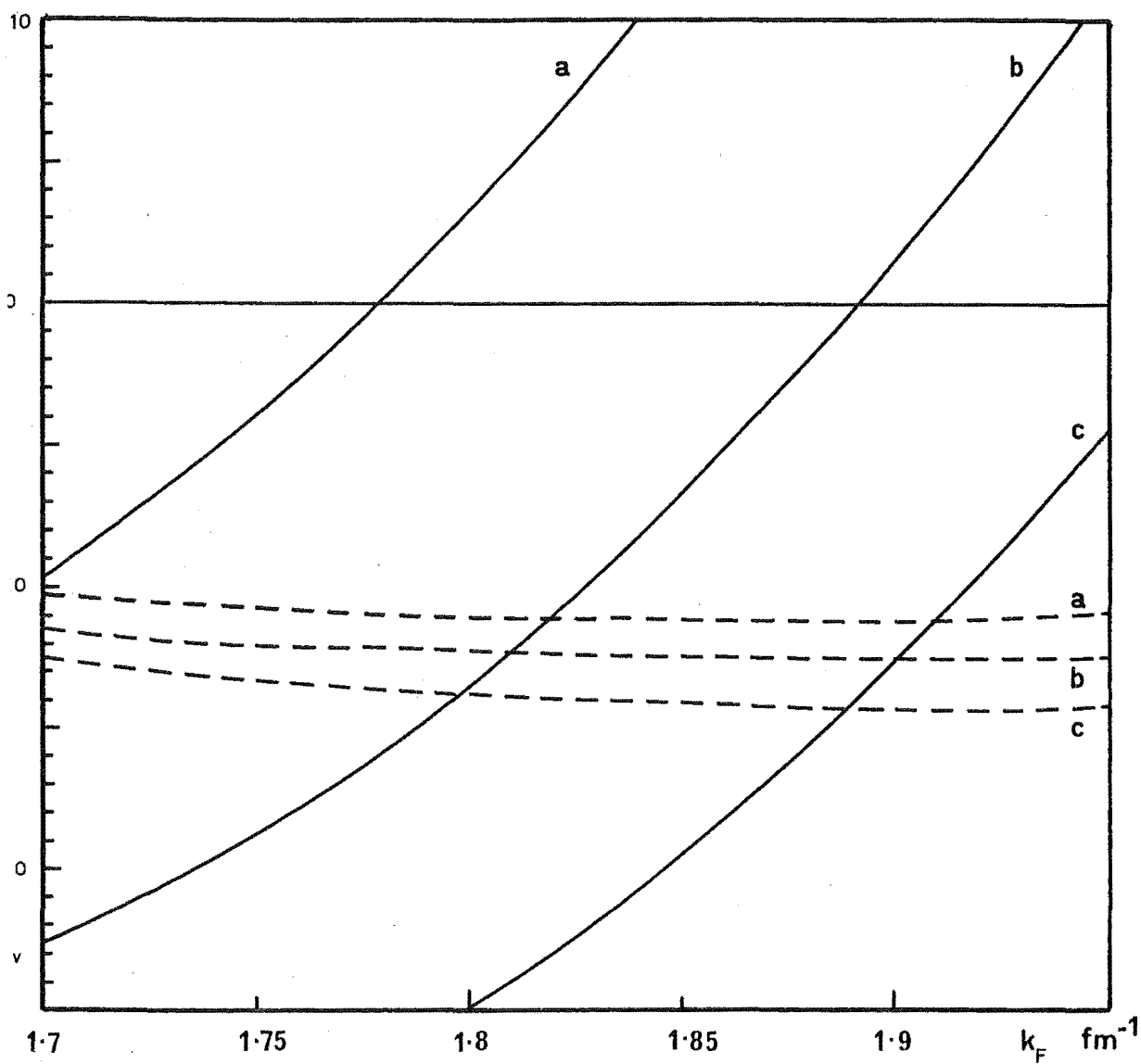
Binding energy per nucleon in nuclear matter with  $\tilde{r} = r + r_c e^{-\beta r}$

(a)  $\beta = 1.0 \text{ fm}^{-1}$

(b)  $\beta = 1.3 \text{ fm}^{-1}$

(c)  $\beta = 1.2 \text{ fm}^{-1}$

FIGURE 2



Variation of the virial near an energy minimum

The solid line gives the value of the expectation value  $F$  given by equation (3.26); the dotted line is the corresponding energy variation.

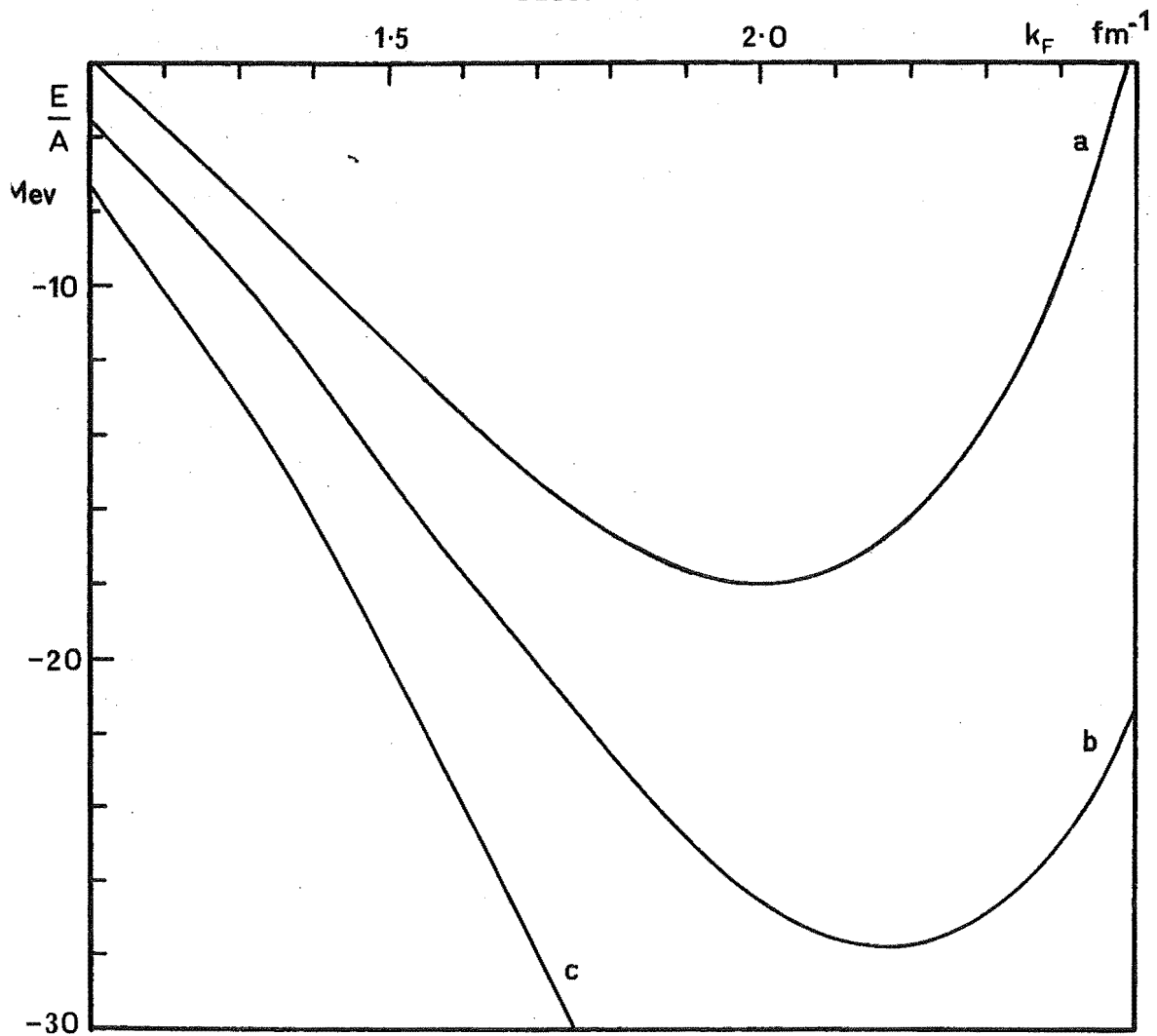
(a)  $\beta = 1.32 \text{ fm}^{-1}$

(b)  $\beta = 1.35 \text{ fm}^{-1}$

(c)  $\beta = 1.37 \text{ fm}^{-1}$



FIGURE 3



Binding energy per nucleon in nuclear matter for different hard-core radii

These curves are calculated with the transformation parameter  
 $\beta = 1.2 \text{ fm}^{-1}$ .

(a)  $r_c = 0.500 \text{ fm}$

(b)  $r_c = 0.490 \text{ fm}$

(c)  $r_c = 0.475 \text{ fm}$

The greater sensitivity of the virial theorem test is illustrated in Figure 2 where we have plotted the energy near its minimum and the value of the functional

$$F = \langle T \rangle - \frac{i}{2\hbar} \left\langle \left[ \sum_k \vec{r}_k \cdot \vec{p}_k, V \right] \right\rangle \quad (3.26)$$

This is to be expected since it is well known that the energy is not very sensitive to wavefunction variations near the minimum and it is for this reason that the use of virial and hypervirial theorems have been suggested as means of improving wavefunctions [37].

The saturation property of nuclear forces due to the hard-core repulsion can be shown if we arbitrarily decrease the hard core radius for a fixed value of  $\beta$ . The results of this are shown in Figure 3. Alternative triplet odd, triplet even and singlet odd potentials with hard-core radii have been given by Gammel, Christian and Thaler, but have not been fitted to all the two-body data. To show that the substitution of these potentials, for which the depths and inverse ranges are given in the following table, cannot improve on the values of energy and density already obtained, it is sufficient to calculate only the energy-density curves for various values of  $\beta$ , since the virial theorem just selects one from a family of such curves. State-dependent transformations are used to allow for different hard-core radii but we retain the single parameter  $\beta$  so that it can, in principle, be determined by the virial theorem.

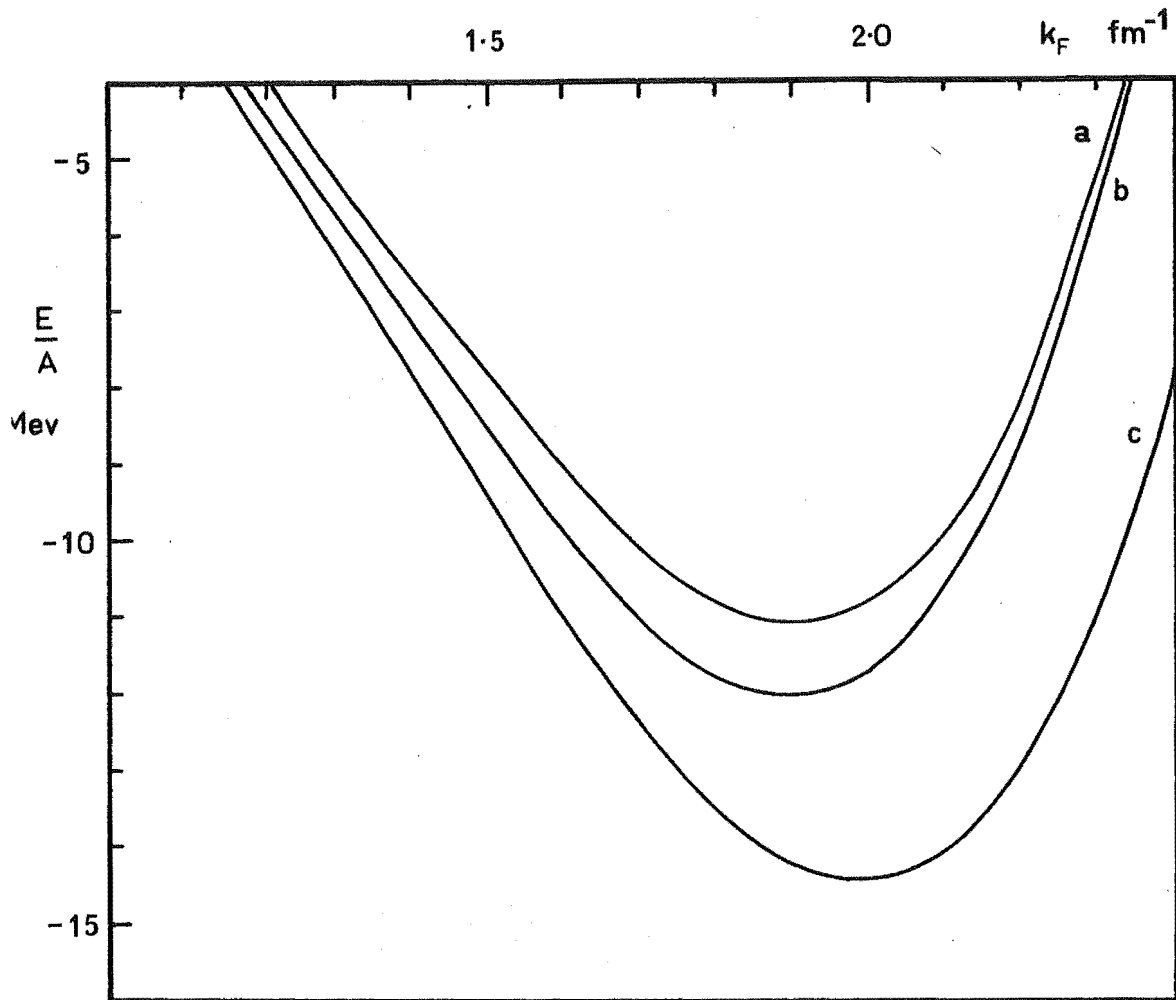
Table 4

GCT central potentials with $r_c = 0.4$ fm		
$V_\alpha^c$	Depth (MeV)	Inverse range ( $\text{fm}^{-1}$ )
$V_1^c$	-100	1.5
$V_2^c$	-2640	2.55
$V_3^c$	-430.2	1.45

In Figure 4 we introduce the softer triplet odd potential, in Figure 5 we replace also the triplet even potential with the reduced hard-core potential, until for Figure 6 all the potentials except the singlet-even have hard-core radii of 0.4 fm. The progressive reduction in hard-core radii leads to an increase in binding energy for a given value of  $\beta$ , except for the curves in Figure 4 where this has been offset by a large decrease in the depth of the triplet-odd potential. For all the potentials tested, it is apparent that an increase in the minimum binding energy is always accompanied by an increase in the equilibrium density. Thus a reduction in the hard-core radii increases the equilibrium density and the results cannot be improved by this means. Potentials with hard-core radii greater than 0.5 fm have not been calculated by Gammel, Christian and Thaler except in the singlet-even case.

The restriction imposed by the choice of the functional form of the transformation  $r \rightarrow \tilde{r}$  limits the extent by which the results may be improved. We have calculated energy-density curves using the transformation of Ristig and Kistler [26] and typical curves are shown in Figure 7.

FIGURE 4

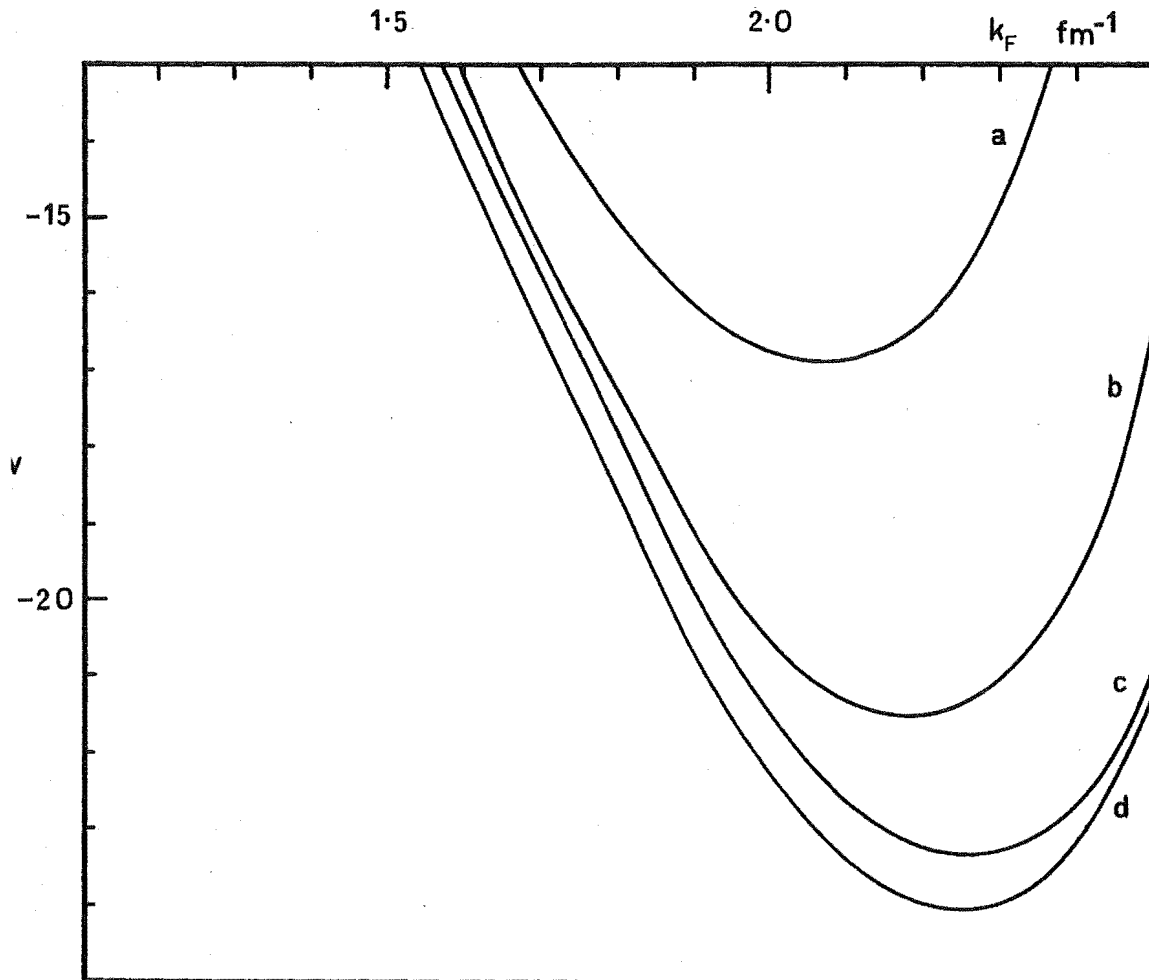


Binding energy per nucleon in nuclear matter.

The potential used is the Gammel, Christian, Thaler potential with the triplet-odd part replaced by the softer-core ( $r_c = 0.4 \text{ fm}$ ) term given in Table 4.  $\beta$  is still taken to be the same for all charge-spin states.

- (a)  $\beta = 1.3 \text{ fm}^{-1}$
- (b)  $\beta = 1.0 \text{ fm}^{-1}$
- (c)  $\beta = 1.2 \text{ fm}^{-1}$

FIGURE 5



Binding energy per nucleon in nuclear matter

with  $V_C^{33}$  and  $V_C^{31}$  replaced by  $r_C = 0.4 \text{ fm}$  terms given in Table 4.

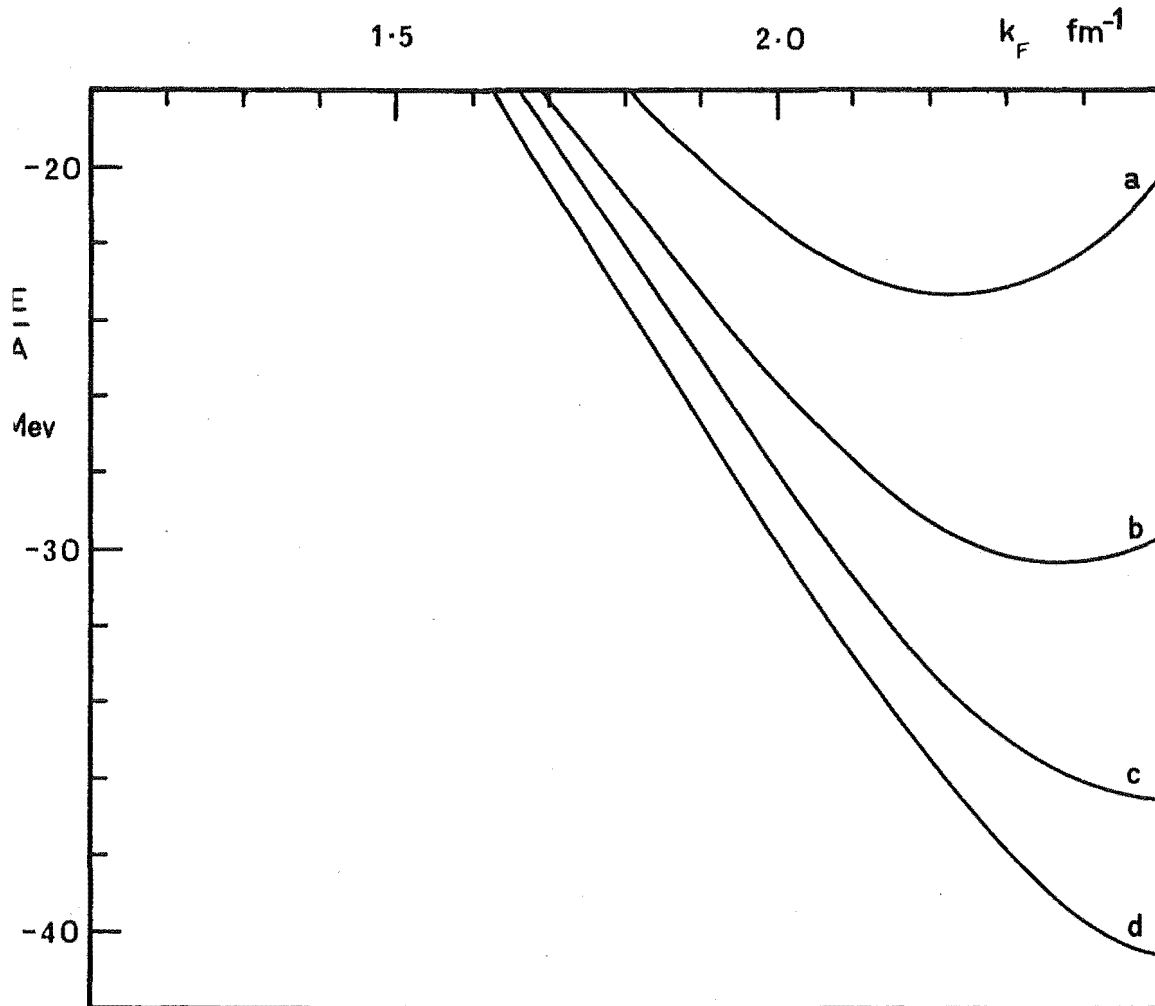
(a)  $\beta = 1.0 \text{ fm}^{-1}$

(b)  $\beta = 1.1 \text{ fm}^{-1}$

(c)  $\beta = 1.4 \text{ fm}^{-1}$

(d)  $\beta = 1.3 \text{ fm}^{-1}$

FIGURE 6



Binding energy per nucleon in nuclear matter

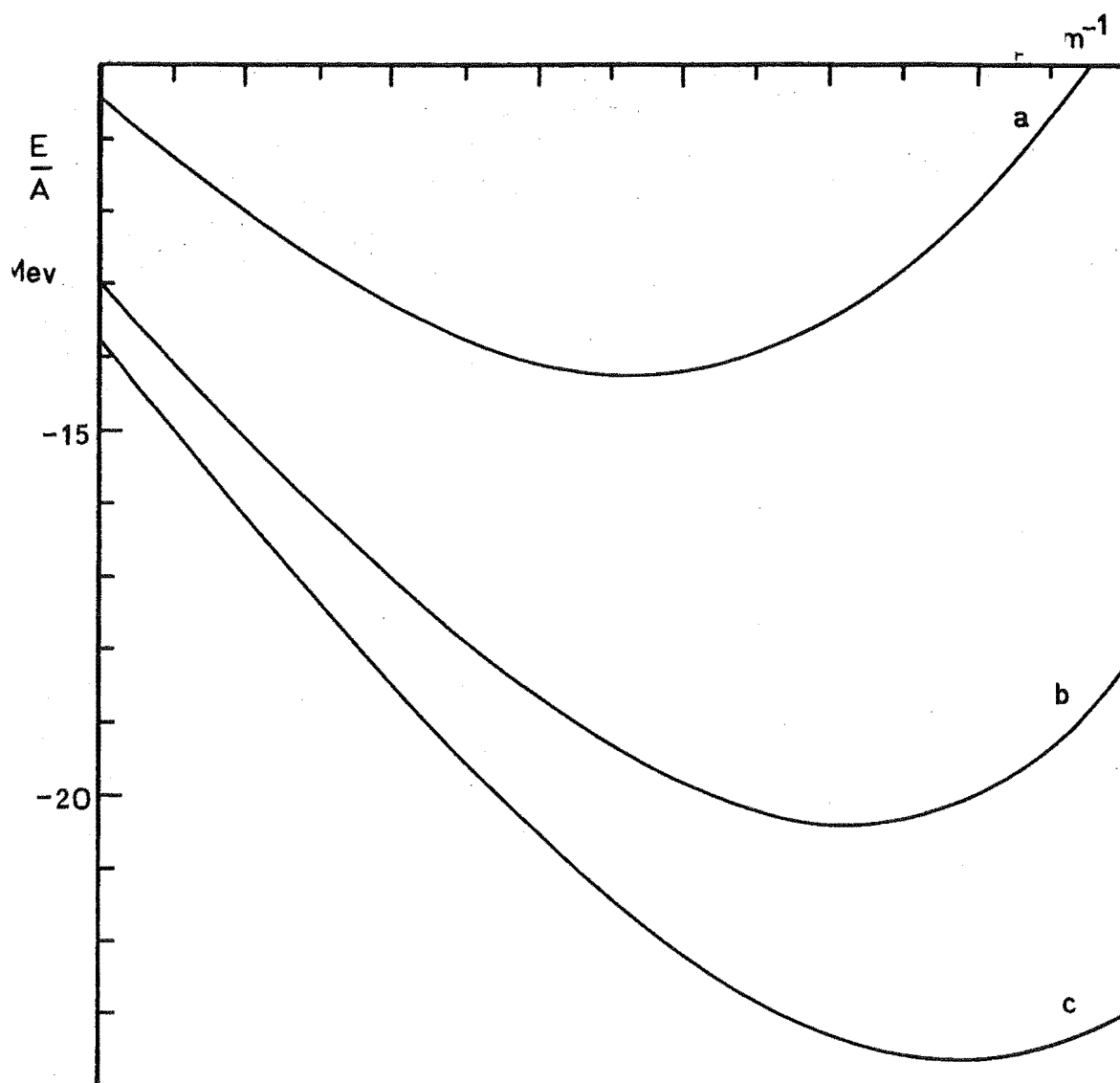
when all terms of the Gammel, Christian Thaler potential except for the singlet-odd term have hard-core radii  $r_c = 0.4$  fm.

(a)  $\beta = 1.0 \text{ fm}^{-1}$

(b)  $\beta = 1.1 \text{ fm}^{-1}$

(c)  $\beta = 1.2 \text{ fm}^{-1}$

(d)  $\beta = 1.3 \text{ fm}^{-1}$



Binding energy per nucleon in nuclear matter

with the radial transformation  $\tilde{r} = r + \frac{1}{\beta} \ln \left\{ 1 + (e^{\beta r_c} - 1)e^{-\beta r} \right\}$

(a)  $\beta = 1.20 \text{ fm}^{-1}$

(b)  $\beta = 1.40 \text{ fm}^{-1}$

(c)  $\beta = 1.67 \text{ fm}^{-1}$

Although the transformed variables (3.20) and (3.21) differ only slightly, (Figure 8), there is a greater difference between their derivatives leading to significant differences in the energy minima and equilibrium densities. If  $\beta$  is determined by the virial theorem we get an energy of  $-23.17$  MeV and density corresponding to  $r_0 = 0.74$  fm for  $\beta = 1.57 \text{ fm}^{-1}$ . These values are too large and would be worse if the energy were minimized with respect to  $\beta$  since this would increase both the energy and the density. Hence in the following discussion and subsequent calculations we will consider only the transformation (3.20).

For nuclear matter we have found that the binding energy per nucleon and the density of nuclear matter obtained by the present method are in reasonable agreement with those obtained by Brueckner using the same static potential. From the energy-density curves we can see the general correlation between the energy and density noted by Coester et al [27] viz an energy increase implies an increase in density. If we regard the transformation solely as a means of removing the hard core, it might be expected that increasing  $\beta$  would be equivalent to reducing the effects of the hard-core since this would allow  $\tilde{r}$  to return rapidly to  $r$  outside the hard-core region. Up to a certain value of  $\beta$  this is the case, but increasing  $\beta$  further reduces the binding energy. The reason for this is that the hard-core repulsion may be regarded as a weak force in many-body systems in the sense that it has a very short range and may be replaced by a softer but larger-range force. Thus the influence of the hard core on the wavefunction extends beyond its radius and the effect of the radial transformation will be to distort the wavefunction in the neighbourhood of the hard-core. In the two-particle case this can be accounted for by a correlation function relating



FIGURE 8

Transformed radial variables

(a)  $\tilde{r} = r + \frac{1}{\beta} \ln \left\{ 1 + (e^{\beta r c} - 1) e^{-\beta r} \right\}$

(b)  $\tilde{r} = r + r c e^{-\beta r}$

(c)  $\tilde{r} = r$

$\tilde{r}$  fm

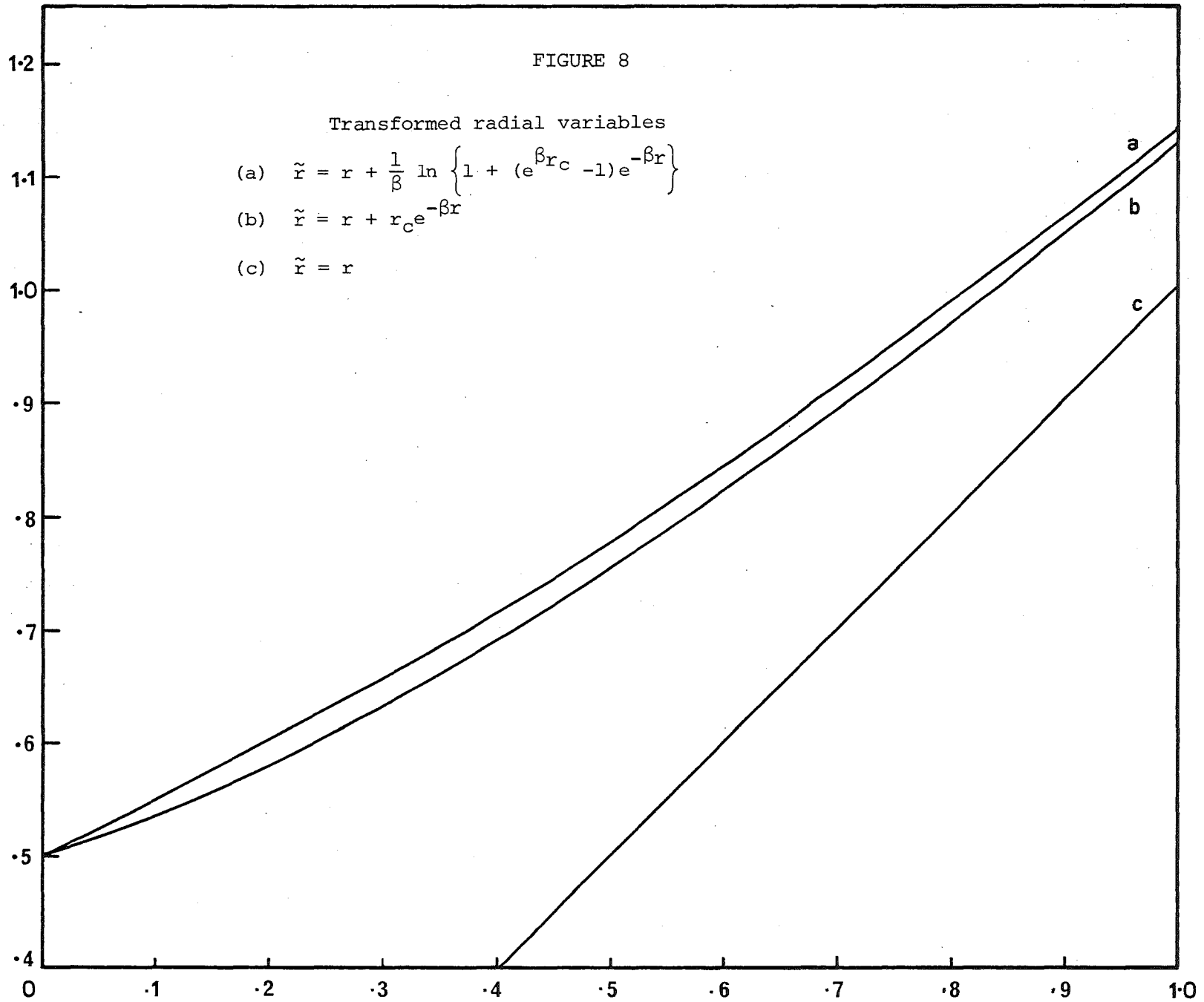
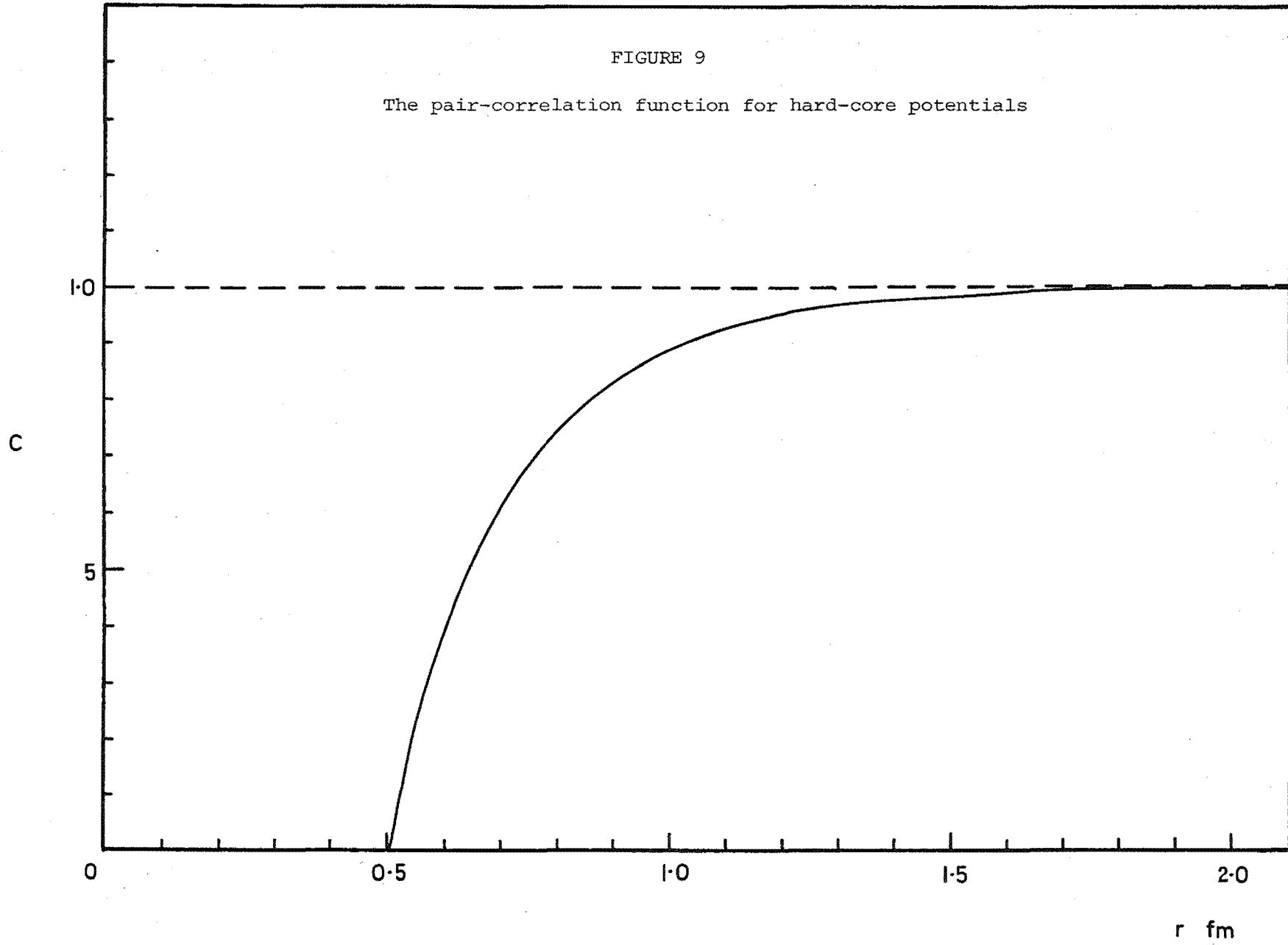


FIGURE 9

The pair-correlation function for hard-core potentials



the correlated and uncorrelated relative wavefunction as

$$\phi(r) = \frac{x}{r} \sqrt{\frac{\partial x}{\partial r}} \tilde{\phi}(x) \quad (3.27)$$

where  $\phi$  is the correlated wavefunction corresponding to a solution of the original Hamiltonian and  $\tilde{\phi}$  the uncorrelated one. The inverse transformation

$$x = U^+ r U \quad (3.28)$$

gives  $x$  as a function of  $r$  so a correlation function  $C(r)$  can be defined by

$$\phi(r) = C(r) \psi(r) \quad (3.29)$$

where  $\psi(r) = \tilde{\phi}(x)$

$$\text{and} \quad C(r) = \frac{x}{r} \sqrt{\frac{\partial x}{\partial r}} \quad (3.30)$$

From Figure 9 it can be seen that the correlation function (3.30) has the features of the correlation factors proposed by Jastrow [17] viz

$$C(r) = 0 \quad r \leq r_c$$

and  $C(r) \rightarrow 1$  when  $r$  is large.

In the correlation function picture we see that large values of  $\beta$  tend to reduce the correlation function and there is a tendency toward weakly-correlated wavefunctions which overestimate the effects of the hard-cores in the Hartree-Fock method. Thus the qualitative effect of varying  $\beta$  is a balance between two tendencies :

- (i) increasing  $\beta$  reduces  $\tilde{r}$  which increases the Yukawa functions

$$\frac{e^{-\mu\tilde{r}}}{\mu\tilde{r}}$$

- (ii) increasing  $\beta$  reduces the correlation functions  $C(r)$ ;

alternatively we can say that it increases the dominant velocity-dependent term, which depends on

$$B^2 = \left( \frac{1}{1 - \beta r_c e^{-\beta r}} \right)^2,$$

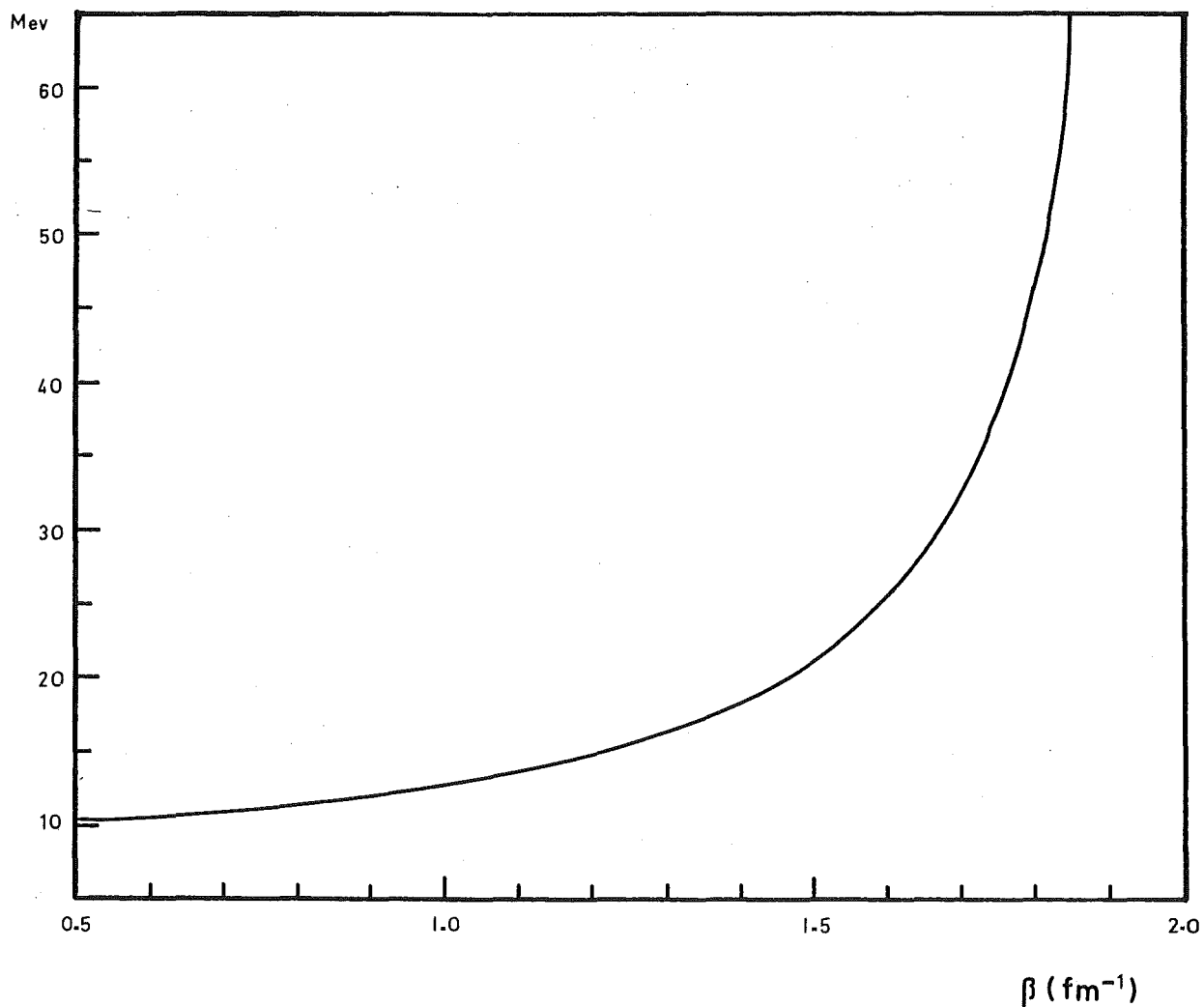
since  $\beta r_c$  is, in the range of interest, less than 1 so for small  $r$   $B^2$  increases with  $\beta$ . The effect (i) is obvious, and to demonstrate that (ii) still holds when we have integrated over the coordinate space, we plot in Figure 10 the contribution of the velocity dependent terms

$$\frac{1}{A} \langle \psi \left| \sum_{ij} \left[ w_{ij} - \sum_{\alpha=1}^4 v_{\alpha}^c(\tilde{r}_{ij}) + v_{\alpha}^t(\tilde{r}_{ij}) s_{ij} \right] \right| \psi \rangle$$

for different values of  $\beta$ .

We have shown that the velocity-dependent potential does reproduce the effect of the repulsive hard-core and that the method can account for some of the two-body correlation. Satisfactory results have been obtained for nuclear matter with the radial transformation

$\tilde{r} = r + r_c e^{-\beta r}$  which we will now use in finite nuclei calculations.



Contribution of the momentum-dependent terms to the binding energy per nucleon in nuclear matter, showing the variation for different values of the transformation parameter  $\beta$ . The quantity shown is the expectation value of the operator  $\sum_{i < j=2}^A (w_{ij} - v(\tilde{r}_{ij}))$ .

## CHAPTER 4

## 4.1 Finite nuclei with velocity-dependent potentials.

The application of the self-consistent field approximation to finite nuclei gives a nuclear model in which there is an ordering and spacing of single-nucleon levels such that properties characteristic of shell-filling and closed-shells may be obtained. The nuclear shell model has been most successful in predicting nuclear properties when the shells are closed or when there is only a small departure from the closed-shell structure. For example, closed-shell nuclei are found to be stable against  $\beta$ -decay and properties such as nuclear spins and magnetic moments can be explained in terms of the behaviour of a few nucleons outside a stable closed-shell. In the following calculations we consider only closed-shell nuclei, for which Ullah and Nesbet [38] have shown the LS-coupling model to be adequate for ground-state calculations. In this model, the single-particle wavefunctions are expressed as

$$\psi_{\alpha}(\vec{r}) = P_{\alpha\ell_{\alpha}}(r) Y_{\ell_{\alpha}}^{m_{\alpha}}(\omega) \chi_{m_{\tau_{\alpha}} \tau_{\alpha}} \xi_{m_{\tau_{\alpha}} \tau_{\alpha}} \quad (4.1)$$

The radial part will be approximated by a finite expansion in terms of harmonic oscillator radial eigenfunctions

$$P_{\alpha\ell}(r) = \sum_n c_n^{\alpha} R_{n\ell}(r) \quad (4.2)$$

The unit of length is taken to be the "oscillator length"

$$b = \sqrt{\frac{\hbar}{m\omega}}$$

giving an energy unit of  $\hbar\omega$ , so the normalized harmonic oscillator

functions are

$$R_{n\ell}(r) = \sqrt{\frac{2n!}{\Gamma(n + \frac{3}{2})}} r^\ell e^{-\frac{1}{2}r^2} L_n^{\ell + \frac{1}{2}}(r^2) \quad (4.3)$$

For a finite nucleus the calculation of the energy is complicated by the fact that the centre of mass of the nucleus is not localized in space and the trial wavefunction used in the independent particle model cannot be separated as a product of wavefunctions for the centre-of mass and the internal motions. This problem arises because the A-particle wavefunction is assumed to be a function of 3A space coordinates, whereas three of these coordinates, describing the centre-of mass motion, are redundant when we wish to calculate the internal properties of a nucleus. Nevertheless a good approximation to the nuclear binding energy may be obtained by subtracting the centre of mass kinetic energy from the Hamiltonian [39] giving an intrinsic Hamiltonian:

$$H = \sum_{i=1}^A \frac{p_i^2}{2m} + \sum_{i<j=2}^A w_{ij} - \frac{1}{2} \left( \frac{\sum_{i=1}^A \vec{p}_i}{Am} \right)^2$$

$$\begin{aligned} \text{Since } \left( \sum_i \vec{p}_i \right)^2 &= \sum_i p_i^2 + 2 \sum_{i<j} \vec{p}_i \cdot \vec{p}_j \\ &= A \sum_i p_i^2 - \sum_{i<j} (\vec{p}_i - \vec{p}_j)^2 \end{aligned}$$

the intrinsic Hamiltonian can also be written as [40]

$$H = \frac{1}{2} \sum_{i \neq j=1}^A \left[ \frac{(\vec{p}_i - \vec{p}_j)^2}{2Am} + w_{ij} \right] \quad (4.4)$$

In equation (2.12) we defined a relative kinetic energy operator

$$t = \frac{p^2}{2m_{\text{red}}}$$

in terms of the relative momentum  $\vec{p} = \frac{1}{2}(\vec{p}_1 - \vec{p}_2)$  and the reduced mass  $m_{\text{red}} = \frac{m}{2}$ .

Therefore

$$t_{ij} = \frac{(p_i - p_j)^2}{4m} \quad (4.5)$$

$$\text{and } H = \frac{1}{2} \sum_{i \neq j=1} \left[ \frac{2}{A} t_{ij} + w_{ij} \right] \equiv \frac{1}{2} \sum_{i \neq j} h_{ij} \quad (4.6)$$

Since  $H$  contains only two-particle operators the total energy is expressible as a sum of two-particle matrix elements:

$$\langle H \rangle = \frac{1}{2} \sum_{\alpha, \beta} \langle \alpha\beta | h_{12} | \alpha\beta \rangle - \langle \alpha\beta | h_{12} | \beta\alpha \rangle \quad (4.7)$$

using the notation  $|\alpha\rangle = \psi_{\alpha}(\vec{r})$ . The two-particle functions  $|\alpha\beta\rangle$  can in principle be expanded in terms of relative and two-particle centre of mass functions [41] by taking a complete set of wavefunctions  $|N\rangle$  for the centre of mass motion and a complete set  $|n\sigma\rangle$  for the relative motion

$$|\alpha\beta\rangle = \sum_{nN\sigma} |N, n\sigma\rangle \langle N, n\sigma | \alpha\beta \rangle \quad (4.8)$$

where  $\sigma$  gives the charge-spin states of the nucleon pair. Since  $h_{12}$  acts only on the relative coordinates the energy depends only on matrix elements of the form

$$\langle \alpha\beta | h_{12} | \lambda\mu \rangle = \sum_N \sum_{nn'} \sum_{\sigma} \langle \alpha\beta | N, n\sigma \rangle \langle n\sigma | h_{12} | n'\sigma \rangle \langle N, n'\sigma | \lambda\mu \rangle$$

We now define an effective interaction  $w_{12}$  by the relation

$$h_{12} = \frac{2}{A} t_{12} + w_{12} = e^{i\Omega_{12}} \left( \frac{2}{A} t_{12} + v_{12} \right) e^{-i\Omega_{12}} \quad (4.10)$$

In the case  $A = 2$  this is identical to that obtained in Chapter 2 so all the conditions specified earlier are still satisfied. In particular we may define a correlation function for the two-particle functions

$$C(r_{12}) = \frac{f_{12}}{r_{12}} \sqrt{\frac{\partial f_{12}}{\partial r_{12}}} \quad (4.11)$$



and the velocity-dependent potential is now

$$w(r) = \frac{2}{Am} \left[ \frac{1}{2} \left\{ (B^2-1) p_r^2 + p_r^2 (B^2-1) \right\} + \ell^2 \left( \frac{1}{\tilde{r}^2} - \frac{1}{r^2} \right) + \frac{\hbar^2}{2} B \frac{\partial^2 B}{\partial r^2} + \frac{3\hbar^2}{4} \left( \frac{\partial B}{\partial r} \right)^2 \right] + v^c(\tilde{r}) + v^t(\tilde{r}) S_{12} \quad (4.12)$$

Using our earlier notation for the correlated and uncorrelated wavefunctions given in (3.29) we can rewrite

$$\langle n\sigma | h_{12} | n'\sigma \rangle = \langle n\sigma | e^{i\Omega_{12}} \left( \frac{2}{A} t_{12} + v_{12} \right) e^{-i\Omega_{12}} | n'\sigma \rangle$$

as 
$$\langle \psi_{n\sigma} | h_{12} | \psi_{n'\sigma} \rangle = \langle \phi_{n\sigma} | \frac{2}{A} t_{12} + v_{12} | \phi_{n'\sigma} \rangle \quad (4.13)$$

where  $\psi_{n\sigma}$  is an uncorrelated wavefunction and  $\phi_{n\sigma}$  a correlated one, and they are related by

$$\phi_{n\sigma} = C \psi_{n\sigma} .$$

In this formulation the connection with the Jastrow correlation function is more direct than that obtained with the previously used effective interactions since the effective interaction with the uncorrelated relative wavefunction gives the same two-particle matrix elements as the realistic interaction with a correlated wavefunction and hence the same total energy. Defining  $h'_{12}$  as

$$h'_{12} = \frac{2}{A} t_{12} + v_{12}$$

we have

$$\langle \psi_{n\sigma} | h_{12} | \psi_{n'\sigma} \rangle = \langle C\psi_{n\sigma} | h'_{12} | C\psi_{n'\sigma} \rangle \quad (4.14)$$

or 
$$h_{12} = Ch'_{12}C \quad (4.15)$$

and 
$$C(r_{12}) = 0 \quad r_{12} < r_c$$

$$C(r_{12}) \rightarrow 1 \quad r_{12} \rightarrow \infty$$

as we have already shown in Chapter 3.

When harmonic oscillator functions are used, the oscillator length  $b$  may be chosen either to give the correct nuclear radius or to minimize the nuclear binding energy. Since  $b$  is a scale factor the energy minimization with respect to  $b$  ensures that the virial theorem is satisfied. This means that the transformation parameter  $\beta$  may be adjusted to give the correct radius or the correct energy. Both of these possibilities will be considered in the following section.

## 4.2 Results for the nucleus $\text{He}^4$

Calculations were carried out for the helium nucleus with the velocity-dependent potentials

$$w = \frac{K}{m} \left[ \frac{1}{2} \left\{ (B^2 - 1) p_r^2 + p_r^2 (B^2 - 1) \right\} + \ell^2 \left( \frac{1}{r^2} - \frac{1}{r^2} \right) + \frac{\hbar^2}{2} B \frac{\partial^2 B}{\partial r^2} + \frac{3\hbar^2}{4} \left( \frac{\partial B}{\partial r} \right)^2 \right] + v^C(\tilde{r}) \quad (4.16)$$

with  $K = 1$  and  $K = \frac{2}{A}$ . The two-particle matrix elements were evaluated using Talmi-Moshinsky transformation brackets [42] and the equivalent radius  $R$  given by

$$R^2 = \frac{5}{3A} \left\langle \sum_i r_i^2 \right\rangle \quad (4.17)$$

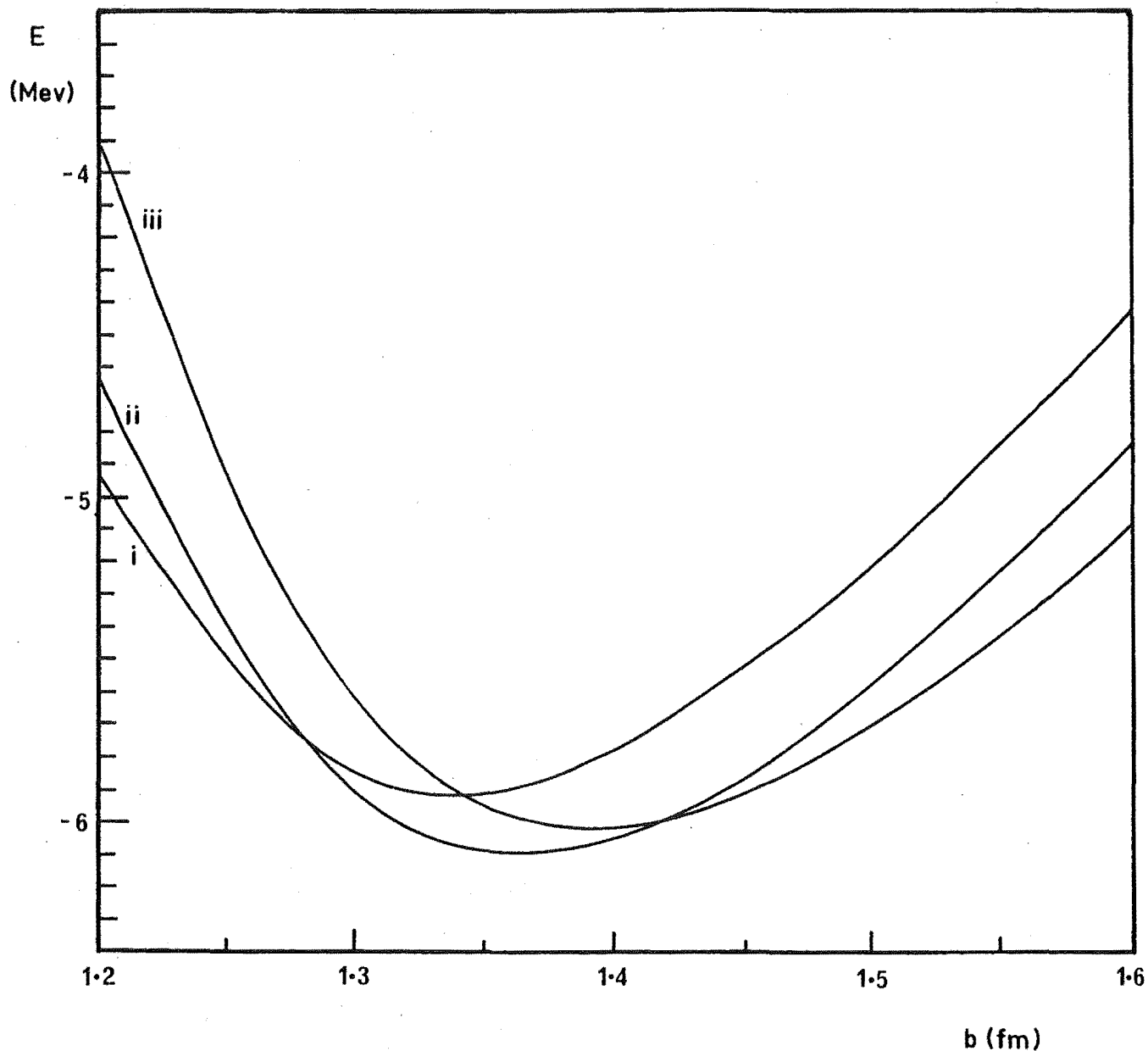
was also calculated.

First calculations were performed assuming the radial functions to be harmonic oscillator functions and with  $K = 1$ . These results are shown in Figure 11. The calculations were repeated using two oscillator functions as a radial basis and the results of these are given in Figure 12. Since the changes in the energy minima due to the additional basis function were very small, the basis was not enlarged further.

The same procedure was applied with  $K = \frac{2}{A}$  and the results of these calculations are given in Figures 13 and 14.

With the potential  $K = 1$ , the correct energy could not be obtained by varying  $\beta$  since the energy was minimized for  $\beta = 1.3 \text{ fm}^{-1}$  at a value of  $-6.1 \text{ MeV}$ . For  $K = \frac{2}{A}$ , the parameter  $\beta$  was adjusted to give an energy of  $-30.1 \text{ MeV}$ , which occurred at  $\beta = 1.62 \text{ fm}^{-1}$ . The energy was minimized with respect to  $b$  at  $b = 1.15 \text{ fm}$  corresponding to a nuclear

FIGURE 11



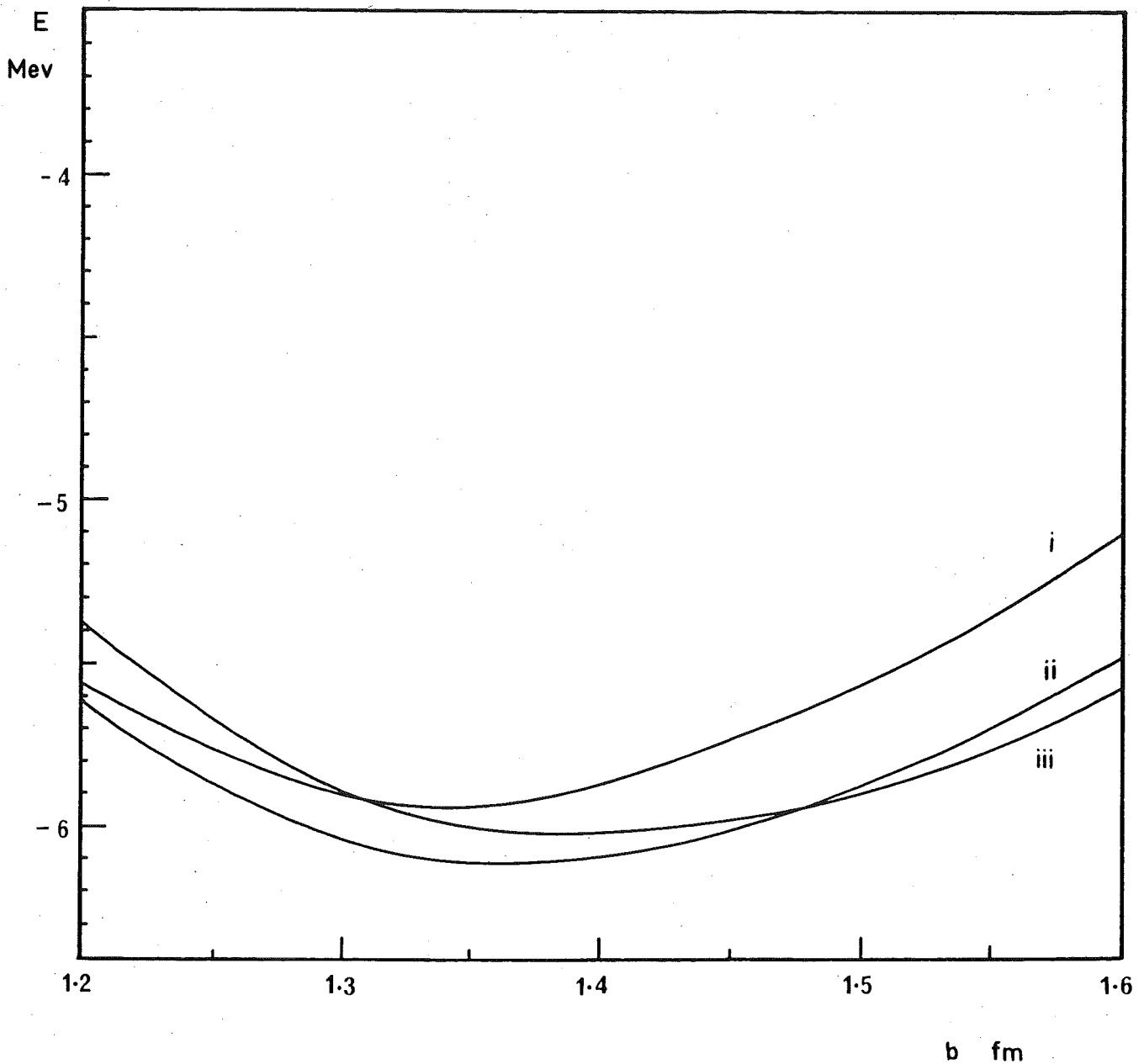
Binding energy of the  $\text{He}^4$  nucleus using the GCT potential with nucleon number-independent effective interactions and the radial wavefunction approximated by a harmonic oscillator function.

$$(i) \beta = 1.2 \text{ fm}^{-1}$$

$$(ii) \beta = 1.3 \text{ fm}^{-1}$$

$$(iii) \beta = 1.4 \text{ fm}^{-1}$$

FIGURE 12



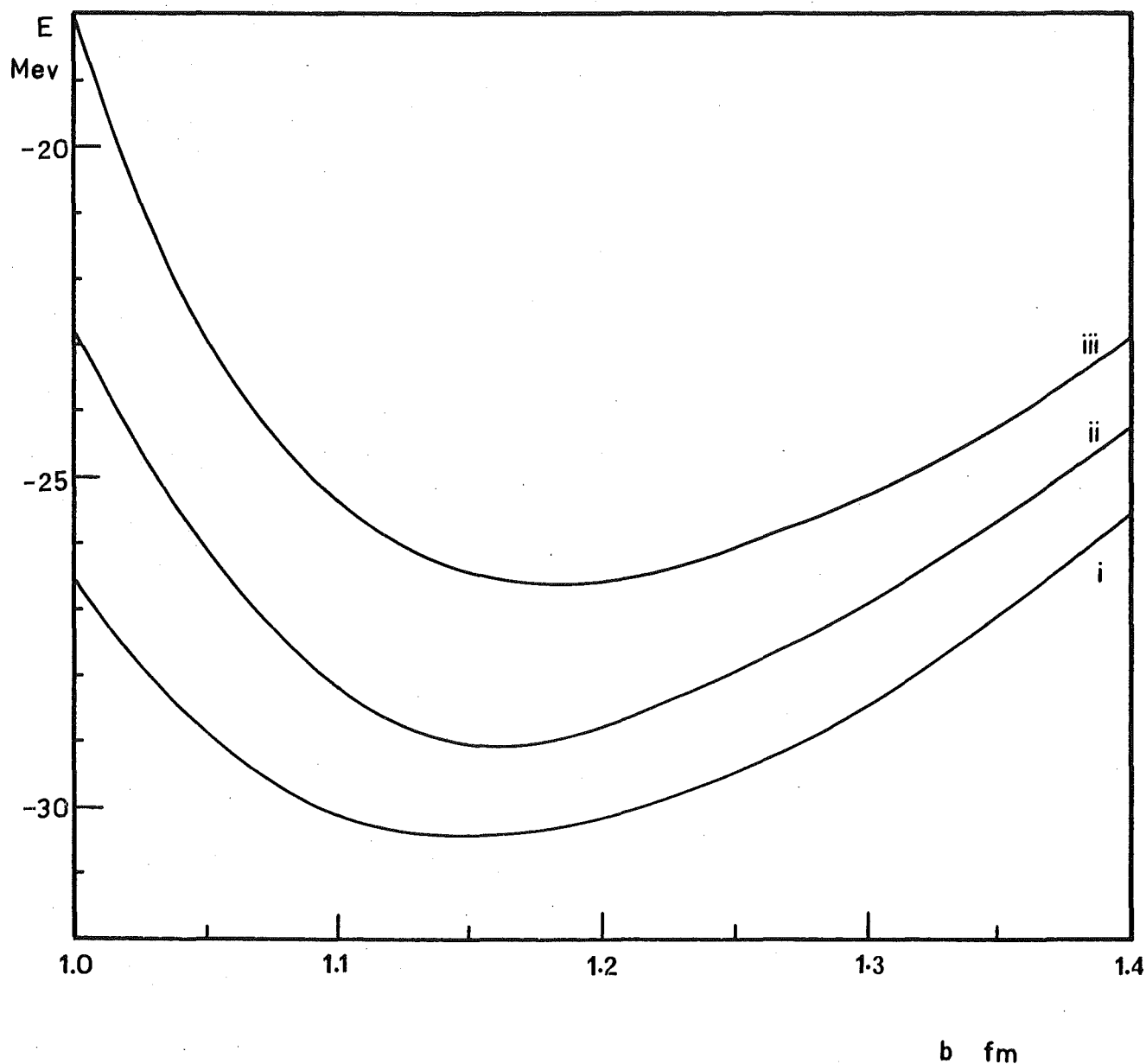
Binding energy of the  $\text{He}^4$  nucleus using the GCT potential with nucleon number-independent effective interactions and the radial wavefunction approximated by a linear combination of two harmonic oscillator functions

$$(i) \beta = 1.2 \text{ fm}^{-1}$$

$$(ii) \beta = 1.3 \text{ fm}^{-1}$$

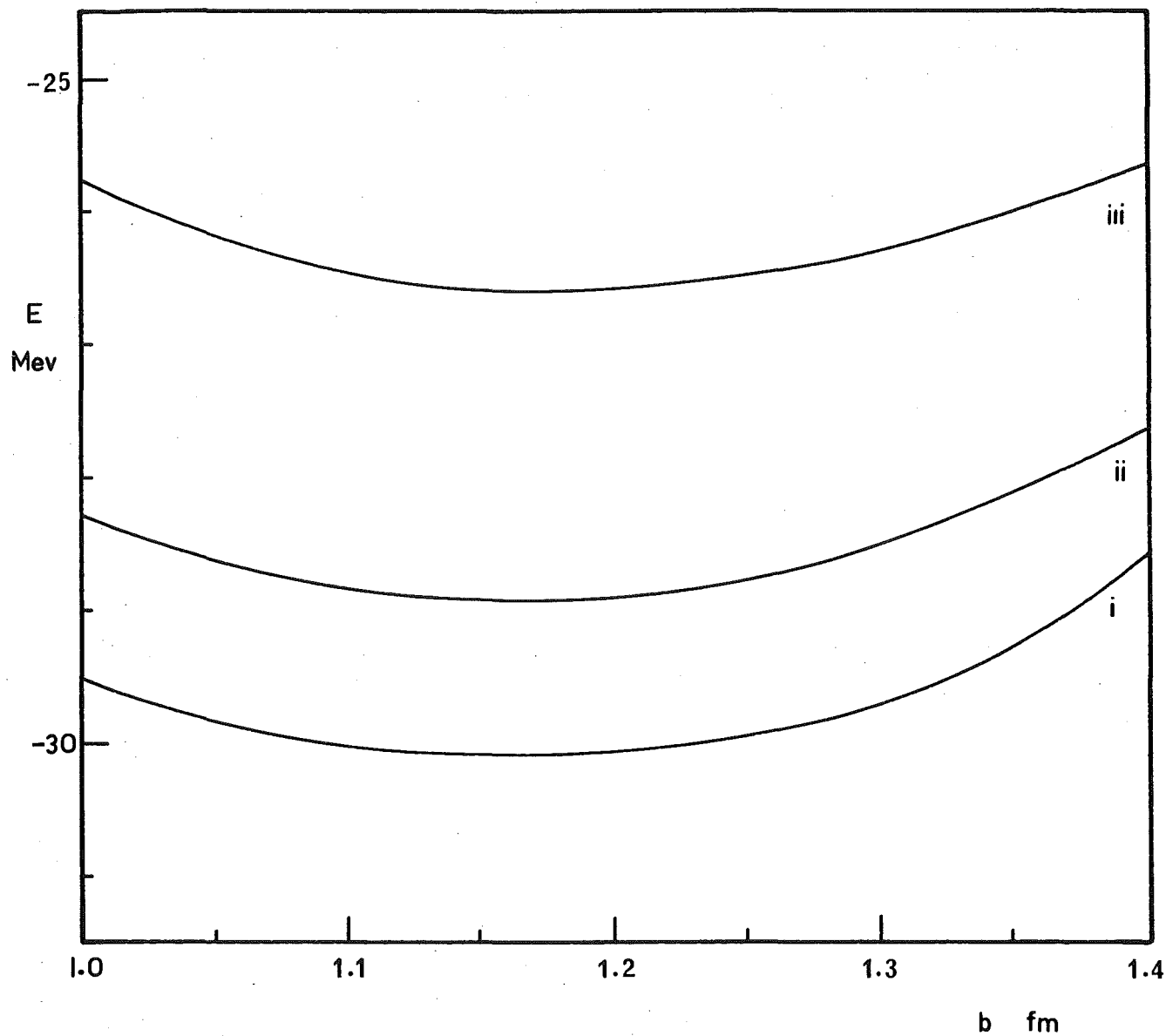
$$(iii) \beta = 1.4 \text{ fm}^{-1}$$

FIGURE 13



Binding energy of the  $\text{He}^4$  nucleus using the GCT potential with effective interactions dependent on the nucleon number; the radial wavefunction is approximated by a harmonic oscillator function.

- (i)  $\beta = 1.62 \text{ fm}^{-1}$
- (ii)  $\beta = 1.63 \text{ fm}^{-1}$
- (iii)  $\beta = 1.64 \text{ fm}^{-1}$



Binding energy of the  $\text{He}^4$  nucleus using the GCT potential with effective interactions dependent on the nucleon number; the radial wavefunction is approximated by a linear combination of two harmonic oscillator functions.

(i)  $\beta = 1.625 \text{ fm}^{-1}$

(ii)  $\beta = 1.630 \text{ fm}^{-1}$

(iii)  $\beta = 1.640 \text{ fm}^{-1}$

radius of 1.82 fm. Fitting the equivalent radius to a value of 2.06 fm gave a minimum energy of -17.3 MeV with  $\beta = 1.68 \text{ fm}^{-1}$ .

The best procedure appears to be fitting the energy to the correct value since the radius obtained is within an acceptable range when compared with other calculations. For a comparison we list the result obtained above with those calculated by Afnan and Tang [43].

Table 5		
	E (MeV)	R (fm)
Present calculation	-30.1	1.82
A	-30.28	1.79
S1	-31.09	1.73
S3	-26.47	1.86

The values listed for the Afnan and Tang potentials A and S1 are those obtained for optimum values of the energy upper bound, and their r.m.s radii have been converted to equivalent radii.

The calculation of too small a nuclear radius for helium is consistent with the result obtained for nuclear matter in which we found that a good value for the energy gave too high a density. We note also that a decrease in the binding energy is accompanied by a decrease in the density. Although we have not obtained agreement with the experimental values of both the energy and the radius, the results compare favourably with these obtained elsewhere for this nucleus [43] and show a considerable improvement over those obtained previously with the Gammel, Christian, Thaler potential.



## CHAPTER 5

## 5.1 Finite nuclei with soft-core potentials

In determining potentials to be used in nuclear structure calculations it is desirable to work with soft-core potentials to simplify subsequent calculations even though this means that the potentials will not fit the high-energy two-nucleon data. Nevertheless it is possible to calculate soft-core potentials which agree to a sufficiently high energy so that they are realistic potentials in the energy range encountered in nuclei. By removing the restriction that a nuclear potential should fit all the two-body data, it may be fitted instead to the properties of light nuclei. Such potentials are those obtained by Afnan and Tang [43] which were fitted to the nuclei  $\text{He}^3$  and  $\text{He}^4$ , and that calculated by Volkov [20], fitted to  $\text{He}^4$  and  $\text{O}^{16}$ .

With this procedure, the difficulty arises that accurate methods of calculating the many-body wavefunctions must be used or the fitting of the data will result in an error in the potential compensating for an error in the approximate wavefunction. The spin-independent effective Hamiltonians of Afnan and Tang are calculated using totally symmetric correlated wavefunctions of the form

$$\psi = \prod_{i < j = 1}^A f(r_{ij}) \quad (5.1)$$

while Volkov has used a product of harmonic-oscillator wavefunctions. The Volkov potential has also been used by Afnan and Tang with their trial wavefunction (5.1) and both this potential and those of Afnan and Tang have been used in  $\text{He}^3$  and  $\text{He}^4$  calculations with a more general trial wavefunction,

$$\underline{\Psi} = \prod_{i < j = 1}^A f(r_{ij}) \Phi \quad (5.2)$$

where  $\Phi$  is a central-field wavefunction, by Fantoni, Panattoni and Rosati [44]. For s-shell nuclei  $\Phi$  was assumed to be the product of a normalized spin function and a radial function which was a superposition of Gaussians.

The principal difficulty in obtaining accurate estimates of the binding energy of light nuclei is in the determination of the radial functions. Since  $\text{He}^4$  has been calculated in all the above references we will consider it in detail in the following section. By working with an s-shell nucleus we can concentrate on an accurate determination of the radial function and distinguish between discrepancies in the results due to unreliable radial functions and those which are essentially due to correlation.

## 5.2 Finite-difference solution of He<sup>4</sup>

Results for the He<sup>4</sup> nucleus have been obtained in references [43], [44] using the Volkov potential which has the form

$$V(\vec{r}) = \left[ V_1 e^{-\left(\frac{r}{r_1}\right)^2} + V_2 e^{-\left(\frac{r}{r_2}\right)^2} \right] (1-m + mP_x) \quad (5.3)$$

where  $P_x$  is the space exchange operator. The depth and range parameters  $V_1, V_2$  and  $r_1, r_2$  and the exchange mixture  $m$  have been approximately fitted to the s-wave scattering length and effective range, and the binding energy and radii of He<sup>4</sup> and O<sup>16</sup>. The resulting parameters are

$$V_1 = - 83.34 \quad \text{MeV} \quad (5.4a)$$

$$r_1 = 1.6 \quad \text{fm} \quad (5.4b)$$

$$V_2 = 144.86 \quad \text{MeV} \quad (5.4c)$$

$$r_2 = 0.82 \quad \text{fm} \quad (5.4d)$$

$$m = 0.6 \quad (5.4e)$$

The single particle functions in the Hartree-Fock approximation for s-shell nuclei are

$$\phi_\alpha(\vec{r}) \equiv \frac{1}{\sqrt{4\pi}} r^{-1} R_\alpha(r) \chi(m_{S\alpha}) \xi(m_{T\alpha}) \quad (5.5)$$

The space exchange operator is related to the charge and spin exchange operators,  $P_\sigma$  and  $P_\tau$ , for totally antisymmetric states by the relation

$$P_x P_\sigma P_\tau = - 1$$

$$\text{or} \quad P_x = - P_\sigma P_\tau \quad (5.6)$$

It is convenient to rewrite the interaction (5.3) as

$$\left[ V_1 e^{-\left(\frac{r}{r_1}\right)^2} + V_2 e^{-\left(\frac{r}{r_2}\right)^2} \right] (1-m + mP_x) \equiv V(r) (a-bP_\sigma P_\tau) \quad (5.7)$$

with  $a = 1-m$  and  $b=m$ . The radial dependence  $V(r)$  can be expressed in a Legendre expansion

$$V(r) = \sum_{\lambda=0}^{\infty} \frac{4\pi}{2\lambda+1} v_\lambda(r_1, r_2) P_\lambda(\cos\omega_{12})$$

where  $\cos\omega_{12} = \frac{\vec{r}_1 \cdot \vec{r}_2}{|\vec{r}_1| |\vec{r}_2|}$  and  $v_\lambda$  for each Gaussian function is calculated in

Appendix 2A. For  $\text{He}^4$  only  $v_0$  is required in the radial Hartree-Fock equation

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} R_\alpha(r) + \sum_{\beta=1}^4 \left[ (a - \delta_{\alpha\beta}^{\sigma\tau}) \int_0^\infty dr' R_\beta^2(r') v_0(r, r') \right] R_\alpha(r) \\ + \sum_{\beta=1}^4 \left[ (b - \delta_{\alpha\beta}^{\sigma\tau}) \int_0^\infty dr' R_\alpha(r) v_0(r, r') R_\beta(r') R_\beta(r) \right] \\ = \epsilon_\alpha R_\alpha(r) \end{aligned} \quad (5.8)$$

where  $\delta_{\alpha\beta}^{\sigma\tau} = \delta(m_{s_\alpha}, m_{s_\beta}) \delta(m_{\tau_\alpha}, m_{\tau_\beta})$

To subtract the centre-of-mass kinetic energy we express it in the form

$$\frac{(\sum_i \vec{p}_i)^2}{2Am} = \frac{-\hbar^2}{2Am} \left( \sum_{i=1}^A \nabla_i^2 + \sum_{i \neq j \neq 1}^A \vec{\nabla}_i \cdot \vec{\nabla}_j \right) \quad (5.9)$$

The first term introduces a factor  $\left(\frac{A-1}{A}\right)$  in the single-particle kinetic energies. We give the general form for the two-particle operator in Appendix 2B.

The equation (5.8) is to be solved in the range  $0 \leq r \leq \infty$ . To convert this to a finite range we use a functional transformation of the radial variable such as that considered by Boys and Handy [45]. If  $r$  is replaced by the variable  $\rho$ , then

$$\frac{d^2}{dr^2} = \left( \frac{d\rho}{dr} \frac{d}{d\rho} \right)^2$$

To simplify the notation we define

$$g \equiv \frac{d\rho}{dr}$$

and obtain

$$\begin{aligned} \frac{d^2}{dr^2} &= g \frac{d}{d\rho} g \frac{d}{d\rho} \\ \text{or} \quad \frac{d^2}{dr^2} &= g^{\frac{3}{2}} \frac{d^2}{d\rho^2} g^{\frac{1}{2}} - \frac{g}{2} \frac{d^2 g}{d\rho^2} + \frac{1}{4} \left( \frac{dg}{d\rho} \right)^2 \end{aligned} \quad (5.10)$$

Substituting new radial functions

$$P_\alpha(\rho) = g^{\frac{1}{2}} R_\alpha(r)$$

and including the centre of mass correction we obtain

$$\left\{ \frac{-\hbar^2}{2m} \left( \frac{A-1}{A} \right) \left[ \frac{d^2}{d\rho^2} - \frac{1}{2g} \frac{d^2 g}{d\rho^2} + \frac{1}{4g^2} \left( \frac{dg}{d\rho} \right)^2 \right] + \frac{Y_\alpha}{g^2}(\rho) + \frac{\epsilon_\alpha}{g^2} \right\} P_\alpha(\rho) + \frac{X_\alpha}{g^2}(\rho) = 0 \quad (5.11)$$

$$\text{where} \quad Y_\alpha(\rho) = \sum_{\beta=1}^4 (a - \delta_{\alpha\beta}^{\sigma\tau} b) \int_0^{\rho_{\max}} \frac{P_\beta^2(\rho') v_0(\rho, \rho') d\rho'}{g^2} \quad (5.12)$$

$$\text{and} \quad X_\alpha(\rho) = \sum_{\beta=1}^4 (b - \delta_{\alpha\beta}^{\sigma\tau} a) \int_0^{\rho_{\max}} \frac{P_\alpha(\rho') v_0(\rho, \rho') P_\beta(\rho')}{g^2} d\rho' P_\beta(\rho) \quad (5.13)$$

The transformation

$$\rho = \frac{r}{1+cr} \quad \text{with} \quad \rho_{\max} = \frac{1}{c}$$

used by Cayford, Fimple and Unger [46] in their finite-difference calculations is taken giving the equation (with  $\hbar^2/m = 1$ )

$$\left[ -\frac{1}{2} \left( \frac{A-1}{A} \right) \frac{d^2}{d\rho^2} + \frac{Y_\alpha(\rho)}{(1-c\rho)^4} - \frac{\epsilon_\alpha}{(1-c\rho)^4} \right] P_\alpha(\rho) + \frac{X_\alpha(\rho)}{(1-c\rho)^4} = 0 \quad (5.14)$$

Following the method given in reference [46] we divide the interval

$0 \leq \rho \leq \frac{1}{c}$  by  $M-1$  equally spaced internal mesh points so the spacing of points is  $h = \frac{1}{Mc}$ . Denoting distances as

$$\rho_k = kh \quad (5.15)$$

and values of functions at the mesh points by

$$P_\alpha(\rho_k) = P_\alpha^k \quad (5.16)$$

gives the equations in finite-difference form

$$\left[ \frac{1}{h^2} + \frac{Y_\alpha^k}{(1-ckh)^4} - \frac{\epsilon_\alpha}{(1-ckh)^4} \right] P_\alpha^k - \frac{1}{2h^2} (P_\alpha^{k-1} + P_\alpha^{k+1}) + \frac{X_\alpha^k}{(1-ckh)^4} = 0 \quad (5.17)$$

where use has been made of the approximation for the second derivative

$$\left( \frac{d^2 P_\alpha}{d\rho^2} \right)_{\rho=\rho_k} \approx \frac{1}{h^2} (P_\alpha^{k-1} - 2P_\alpha^k + P_\alpha^{k+1})$$

The boundary conditions are

$$P_\alpha^0 = P_\alpha^M = 0 \quad (5.18)$$

so the direct and exchange integrals can be expressed as

$$Y_\alpha^k = h \sum_{\beta=1}^4 (a-\delta_{\alpha\beta}^{\sigma\tau}) \sum_{j=1}^{M-1} \frac{(P_\beta^j)^2 v_0(kh, jh)}{(1-cjh)^4}$$

$$X_\alpha^k = h \sum_{\beta=1}^4 (b-\delta_{\alpha\beta}^{\sigma\tau}) \sum_{j=1}^{M-1} \frac{P_\alpha^j P_\beta^j v_0(kh, jh) P_\beta^k}{(1-cjh)^4}$$

using the trapezoidal rule. Similarly the normalization constraint enters as

$$\sum_{j=1}^{M-1} \frac{(P_\alpha^j)^2}{(1-cjh)^4} - \frac{1}{h} = 0 \quad (5.19)$$

By redefining  $P_\alpha^M$  to be the eigenvalue  $\epsilon_\alpha$ , (5.17) is rewritten as

$$\left[ \frac{1}{h^2} + \frac{Y_\alpha^k}{(1-ckh)^4} - \frac{P_\alpha^M}{(1-ckh)^4} \right] P_\alpha^k - \frac{1}{2h^2} (P_\alpha^{k-1} + P_\alpha^{k+1}) + \frac{X_\alpha^k}{(1-ckh)^4} = 0 \quad (5.20)$$

Then the equations (5.19) and (5.20) can be solved by a generalized Newton-Raphson iteration

$$\vec{P}_\alpha^{(n+1)} = \vec{P}_\alpha^{(n)} - [J^{(n)}]^{-1} \vec{F}_\alpha^{(n)} \quad (5.21)$$

where

- (i)  $\vec{P}_\alpha^{(n)}$  is the vector of  $P_\alpha^k$  values at the  $n$ th iteration  
(ii)  $J_n$  is the Jacobian matrix whose elements are

$$J_{\ell m}^{(n)} = \left[ \frac{\partial f_\alpha^\ell}{\partial P_\alpha^m} \right]^{(n)}$$

and (iii)  $\vec{F}_\alpha^{(n)}$  is the vector of values  $f_\alpha^k$  of the equations (5.19) and (5.20) at the  $n$ th iteration. The Jacobian matrix has an almost tridiagonal form and algorithms for rapid manipulation of such matrices have been developed by Cayford, Fimple and Unger [46].

The matrix elements of the Jacobian matrix for  $\text{He}^4$  are given below

$$\begin{aligned} J_{kk'} &= \frac{1}{h^2} + \frac{y_\alpha^k}{(1-ckh)^4} - \frac{P_\alpha^m}{(1-ckh)^4} & k = k' \\ &= \frac{1}{2h^2} & k = k' \pm 1 \\ &= \frac{2P_\alpha^{k'}}{(1-ck'h)^4} & k = M \\ & & k' = 1, \dots, M-1 \\ &= \frac{P_\alpha^k}{(1-ckh)^4} & k' = M \\ & & k = 1, \dots, M-1 \end{aligned}$$

### 5.3 Results and discussion.

The Newton-Raphson iteration was started with harmonic oscillator functions as approximations to the solutions of the radial equations (5.17). To facilitate convergence the harmonic oscillator potential

$$U(r) = -V_0 + \frac{1}{2} m\omega^2 r^2$$

was introduced with a tracking parameter  $\eta$  so that the radial equation became

$$\left[ \frac{1}{h^2} + \frac{\eta Y_{\alpha}^k}{(1-ckh)^4} - \frac{(1-\eta)V_0}{(1-ckh)^4} + \frac{(1-\eta)k^2 h^2}{2(1-ckh)^4} - \frac{P_{\alpha}^M}{(1-ckh)^4} \right] P_{\alpha}^k - \frac{1}{2h^2} (P_{\alpha}^{k-1} + P_{\alpha}^{k+1}) + \frac{\eta X_{\alpha}^k}{(1-ckh)^4} = 0$$

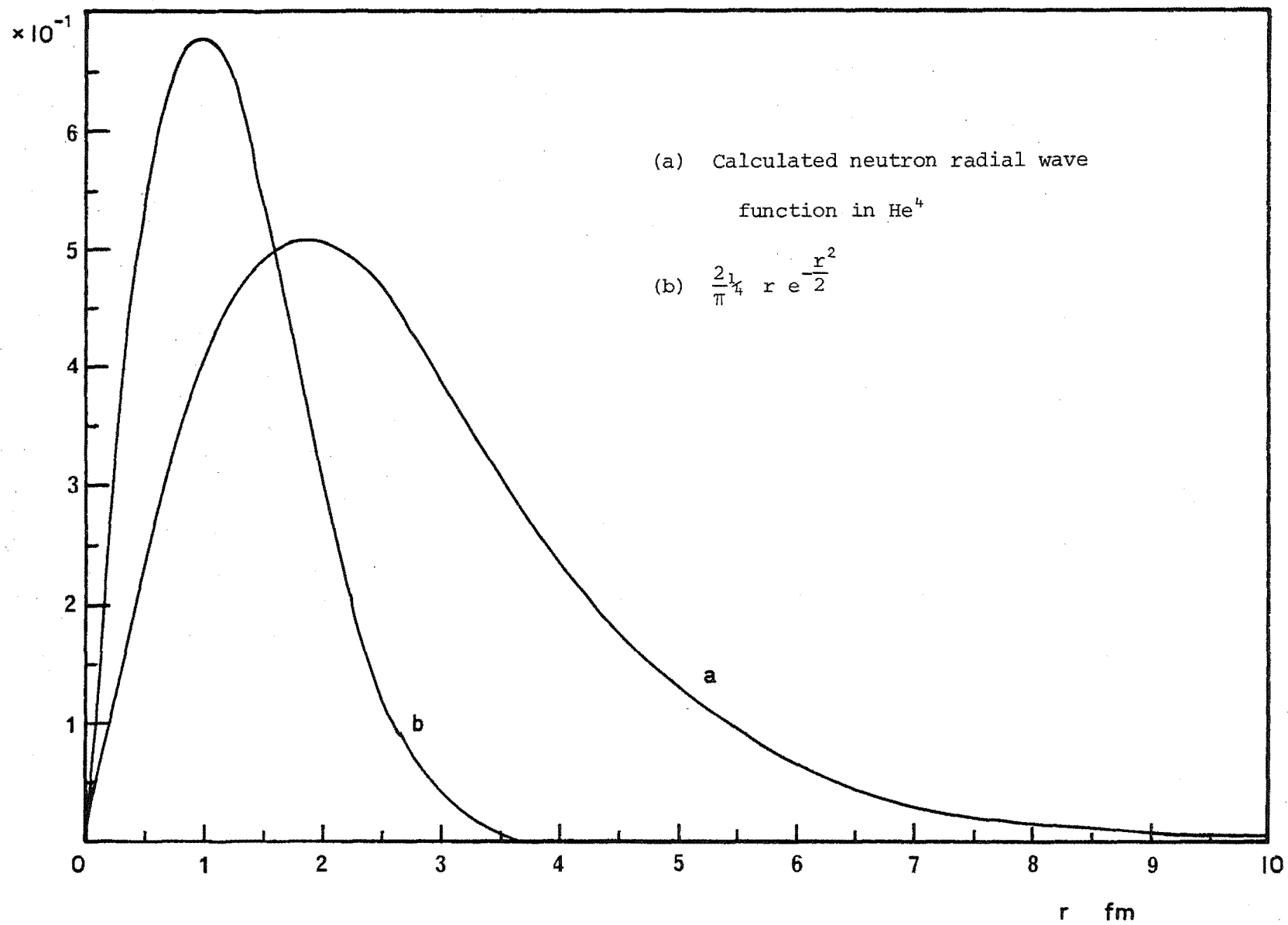
and  $\eta$  was slowly varied from 0 to 1. In addition the coulomb force was included to give different neutron and proton energies.

The calculated wavefunction is shown in Figure 15. This gave an energy of -29.19 MeV, an improvement of 1.18 MeV on the energy obtained by Volkov but not quite as low as those obtained by correlated wavefunction methods.

It is apparent from Figure 15 that a single harmonic oscillator function is too sharply peaked to be a good approximation to the radial wavefunction. To compensate for this, we would expect the Volkov potential to fall off slowly with distance since it must bind nucleons whose wavefunctions are strongly localized. This feature has also been pointed out by Afnan and Tang [43] who attribute the large value obtained for the radius to the long-range of the Volkov potential.



FIGURE 15



Calculating the energy with the trial function (5.1) they obtained upper and lower bounds of -29.95 MeV and -33.86 MeV. The calculations by Fantoni et al [44] take, as the zeroth-order approximation, trial wavefunctions of Gaussian form. The results are then improved by including higher-order terms introduced by the correlation function. The correlation factors  $f$  in (5.2) are used to define new functions  $h(r)$  by

$$f(r) = \sqrt{1-h(r)}$$

and the order  $n$  in Table 6 is the maximum number of  $h$  factors which occur as a product in the energy integral. Since their trial radial function is a crude approximation to the true wavefunction the zeroth-order approximation is poor. In Table 6 we list their results for several orders  $n$  to see where our calculated energy fits in.

TABLE 6	
Order	Energy (MeV)
0	-24.177
1	-26.701
2	-28.409
Present calculation	-29.191
3	-29.230
4	-29.467
5	-29.491
6	-29.490

We can conclude that, at least up to order 2, the correlation function is serving only to improve the crude original approximation for the radial functions, since we have obtained an energy close to their third-order one without introducing explicit dependence on the interparticle distances in our trial wavefunction. Hence the zeroth-order approximation can be considerably improved by just improving the accuracy with which the central field wavefunction is calculated, either by using more flexible trial radial functions or by solving the equations numerically. Ultimately however, the wavefunction should contain a correlation function depending on the nucleon separations as the table above illustrates how this can produce good results even with crude approximations for the central field wavefunction.

## CHAPTER 6

## 6.1 Low-energy two-nucleon phenomena

The only bound two-nucleon system is the deuteron, which consists of a neutron and a proton. Experimentally it is found that the spins of the neutron and proton are coupled to give a total spin 1 and that the magnetic moment of the deuteron is approximately the sum of the neutron and proton magnetic moments. Since there is little orbital contribution to the magnetic moment the deuteron ground state is principally a  ${}^3S_1$  state. The existence of a non-zero quadrupole moment means that it cannot be solely an S-state and the introduction of a tensor force in the two-nucleon potential provides the required admixture of D-state to account for this. We therefore consider the  $({}^3S_1 + {}^3D_1)$  - ground-state of deuteron with a potential

$$V(\vec{r}) = V_c(r) + V_t(r)S_{12} \quad (6.1)$$

where  $S_{12}$  is the tensor force operator defined previously, and  $V_c$  and  $V_t$  are as yet undetermined functions of  $r$ . In terms of the general state-dependent potentials used earlier, we see that only the triplet-even component is given by solving the deuteron problem. This problem has been treated by Feshbach and Schwinger [21] by a variation-iteration method in which the potential parameters were only partly determined by the properties of deuteron. Assuming potentials of Yukawa shape the potentials are parametrized as

$$V_c(r) = V_c^0 \frac{e^{-r/r_c}}{(r/r_c)} \quad (6.2a)$$

$$\text{and } V_t(r) = V_t^0 \frac{e^{-r/r_t}}{(r/r_t)} \quad (6.2b)$$

The variation-iteration method used the binding energy and quadrupole moment of the deuteron to determine the two depth parameters,  $V_C^0$  and  $V_T^0$ , while leaving the range parameters free. This means that the computations must be carried out for a range of values of  $r_C$  and  $r_T$ , and further calculations are necessary to see whether the potentials yield correctly other properties of the neutron-proton system.

The binding energy of the deuteron is known experimentally to be

$$|B.E.| = 2.22452 \text{ MeV} \quad (6.3)$$

and the quadrupole moment

$$Q = 2.37 \times 10^{-27} \text{ cm}^2 \quad (6.4)$$

Less well-determined is the percentage D-state derived from the deuteron magnetic moment. This is estimated as

$$P_D = 3 \pm 1 \% \quad (6.5)$$

where the large uncertainty is due mainly to relativistic effects and meson-theoretic corrections. At low energies (less than  $\sim 10$  MeV), nucleon-nucleon scattering is characterized by the scattering length and effective range. For low energy neutron-proton scattering the scattering length and effective range are related through the deuteron binding energy so we need consider only one of these; we take the effective range

$$\rho = 1.73 \pm 0.04 \text{ fm} \quad (6.6)$$

With the additional data (6.5) and (6.6) we can, in principle, determine all the potential parameters. Earlier methods for determining potentials have involved a large number of systematic computations to

fit some or all of the above data, since they have treated some or all of the parameters as free parameters. In the following we give a set of differential and integral equations which can be solved simultaneously to yield all the potential parameters.

## 6.2 Calculation of a neutron-proton potential.

The Schrödinger equation for the problem in relative coordinates is

$$\left[ \frac{-\hbar^2}{m} \nabla^2 + v(\vec{r}) \right] \psi(\vec{r}) = E \psi(\vec{r}) \quad (6.7)$$

where  $m$  is the nucleon mass (cf equation (2.2) where  $m$  is the reduced mass). For the ( ${}^3S_1 + {}^3D_1$ )-state  $\psi$  may be expressed as

$$\psi(\vec{r}) = \frac{1}{\sqrt{4\pi}} \left[ \frac{u_1(r)}{r} + \frac{1}{\sqrt{8}} S_{12} \frac{u_2(r)}{r} \right] \chi_m \quad (6.8)$$

where  $\chi_m$  are the triplet spin eigenfunctions

$$\begin{aligned} \chi_1 &= \alpha(1)\alpha(2) \\ \chi_0 &= \frac{1}{\sqrt{2}} \left[ \alpha(1)\beta(2) + \alpha(2)\beta(1) \right] \\ \chi_{-1} &= \beta(1)\beta(2) \end{aligned}$$

( $\alpha, \beta$  are the customary spin-up and spin-down eigenfunctions of a single nucleon) and the radial functions  $u_1(r)$  and  $u_2(r)$  are solutions of the coupled differential equations

$$-\frac{\hbar^2}{m} \frac{d^2}{dr^2} u_1(r) + \left[ V_C(r) - E \right] u_1(r) + \sqrt{8} V_t(r) u_2(r) = 0 \quad (6.9)$$

$$\frac{-\hbar^2}{m} \frac{d^2}{dr^2} u_2(r) + \frac{6\hbar^2}{m r^2} u_2(r) + \left[ V_C(r) - 2V_t(r) - E \right] u_2(r) + \sqrt{8} V_t(r) u_1(r) = 0 \quad (6.10)$$

The radial function  $u_1$  corresponds to the S-state and  $u_2$  to the D-state.

The normalization has still to be determined so we choose it to be

$$u_1^2 + u_2^2 \rightarrow e^{-2\alpha r} \quad \text{as } r \rightarrow \infty \quad (6.11)$$

$$\text{where } \alpha = \sqrt{\frac{m|E|}{\hbar^2}} \quad (6.12)$$

We re-express (6.11) as

$$\left. \begin{aligned} u_1 &= N_1 e^{-\alpha r} \\ & \quad r \rightarrow \infty \\ u_2 &= N_2 e^{-\alpha r} \\ & \quad r \rightarrow \infty \end{aligned} \right\} N_1^2 + N_2^2 = 1 \quad (6.13)$$

With the above normalization we have the integral equation for  $u_1$  and  $u_2$  :

$$2 \int_0^{\infty} \left| e^{-2\alpha r} - (u_1^2 + u_2^2) \right| dr = \rho \quad (6.14)$$

Equation (6.14) is the expression for the triplet effective range  $\rho$  whose numerical value is given in (6.6). The percentage D-state is given by

$$\int_0^{\infty} \left[ u_2(r) \right]^2 dr = p_D \int_0^{\infty} \left[ u_1^2(r) + u_2^2(r) \right] dr, \quad (6.15a)$$

$$\text{and we take } p_D = 0.039. \quad (6.15b)$$

The quadrupole moment  $Q$  satisfies the equation

$$\frac{\sqrt{2}}{10} \int_0^{\infty} \left[ u_1(r) - \frac{1}{2\sqrt{2}} u_2(r) \right] u_2(r) r^2 dr = Q \int_0^{\infty} [u_1^2(r) + u_2^2(r)] dr \quad (6.16)$$

Since the nuclear force is short-ranged we solve the coupled equations (6.9) and (6.10) in the range  $0 \leq r \leq R$  with boundary conditions

$$u_1(0) = u_2(0) = 0 \quad (6.17)$$

$$u_1(R) = N_1 e^{-\alpha R} \quad (6.18a)$$

$$u_2(R) = N_2 e^{-\alpha R} \quad (6.18b)$$

The calculations are carried out for a range of values of  $R$  giving potentials which all agree with the specified data. The interval  $[0, R]$  is divided into  $M$  intervals of equal length  $\frac{R}{M}$  and the points designated

$$r_k = \frac{kR}{M} \quad k = 0, 1, \dots, M$$



At each point

$$u_i^k \equiv u_i(r_k)$$

but  $u_i^0 = 0$  so we consider only the  $u_i^k$  with  $k = 1, 2, \dots, M$ . Taking the

Yukawa shape potentials

$$V_c(r) = V_c^0 r_c \frac{e^{-\left(\frac{r}{r_c}\right)}}{r}$$

$$V_t(r) = V_t^0 r_t \frac{e^{-\left(\frac{r}{r_t}\right)}}{r}$$

we define the vector of unknowns  $P_K$  ( $K = 1, 2, \dots, 2M+4$ ) by

$$P_K \equiv u_\ell^k \quad k = 1, 2, \dots, M-1 ; \ell = 1, 2 \quad (6.19a)$$

where  $K = \ell + 2(k-1)$ , so  $1 \leq k \leq M-1$  gives  $1 \leq K \leq 2M-2$

$$P_{2M-1} \equiv N_1 \quad (6.19b)$$

$$P_{2M} \equiv N_2 \quad (6.19c)$$

$$P_{2M+1} \equiv V_c^0 \quad (6.19d)$$

$$P_{2M+2} \equiv r_c \quad (6.19e)$$

$$P_{2M+3} \equiv V_t \quad (6.19f)$$

$$P_{2M+4} \equiv r_t \quad (6.19g)$$

With units so that  $\frac{\hbar^2}{m} = 1$ , and with interval length  $h = \frac{R}{M}$ , we solve for

the  $2M + 4$  unknowns from the following equations.

$$\begin{aligned} & -\frac{1}{h^2} (P_{K-2} + P_{K+2}) + \left[ \frac{2}{h^2} + P_{2M+1} P_{2M+2} \frac{e^{-kh/P}}{kh} \right] P_K \\ & + \sqrt{8} P_{2M+3} P_{2M+4} \frac{e^{-kh/P}}{kh} P_{K+1} = 0 \text{ when } \ell=1 \text{ and } 1 \leq k \leq M-2 \quad (6.20a) \end{aligned}$$

$$\begin{aligned} & -\frac{1}{h^2} (P_{K-2} + P_{K+2}) + \left[ \frac{2}{h^2} + \frac{6}{k^2 h^2} P_{2M+1} P_{2M+2} \frac{e^{-kh/P}}{kh} - 2 P_{2M+3} P_{2M+4} \frac{e^{-kh/P}}{kh} \right] P_K \\ & + \sqrt{8} P_{2M+3} P_{2M+4} \frac{e^{-kh/P}}{kh} P_{K-1} = 0 \text{ when } \ell=2 \text{ and } 1 \leq k \leq M-2 \quad (6.20b) \end{aligned}$$

$$\frac{P_{K-2}}{h^2} - \frac{P_{2M-1} e^{-\alpha R}}{h^2} + \left[ \frac{2}{h^2} + P_{2M+1} P_{2M+2} \frac{e^{-kh/P} 2^{M+2}}{kh} - E \right] P_K$$

$$+ \sqrt{8} P_{2M+3} P_{2M+4} \frac{e^{-kh/P} 2^{M+4}}{kh} P_{K+1} = 0 \quad (\ell=1; k=M-1) \rightarrow (K=2M-3) \quad (6.21a)$$

$$\frac{P_{K-2}}{h^2} - \frac{P_{2M} e^{-\alpha R}}{h^2} + \left[ \frac{2}{h^2} + \frac{6}{k^2 h^2} + P_{2M+1} P_{2M+2} \frac{e^{-kh/P} 2^{M+2}}{kh} - 2 P_{2M+3} P_{2M+4} \frac{e^{-kh/P} 2^{M+4}}{kh} - E \right] P_K$$

$$+ \sqrt{8} P_{2M+3} P_{2M+4} \frac{e^{-kh/P} 2^{M+4}}{kh} P_{K-1} = 0 \quad (\ell=2; k=M-1) \rightarrow (K=2M-2) \quad (6.21b)$$

$$- \frac{P_{K-2}}{h^2} - \frac{P_{2M-1} e^{-\alpha R} e^{-\alpha h}}{h^2} + \left[ \frac{2}{h^2} + P_{2M+1} P_{2M+2} \frac{e^{-kh/P} 2^{M+2}}{kh} - E \right] P_{2M-1} e^{-\alpha R}$$

$$+ \sqrt{8} P_{2M+3} P_{2M+4} \frac{e^{-kh/P} 2^{M+4}}{kh} P_{2M} e^{-\alpha R} = 0 \quad (\ell=1; k=M) \rightarrow (K=2M-1) \quad (6.22a)$$

$$- \frac{P_{K-2}}{h^2} - \frac{P_{2M} e^{-\alpha R} e^{-\alpha h}}{h^2} + \left[ \frac{2}{h^2} + \frac{6}{k^2 h^2} + P_{2M+1} P_{2M+2} \frac{e^{-kh/P} 2^{M+2}}{kh} - 2 P_{2M+3} P_{2M+4} \frac{e^{-kh/P} 2^{M+4}}{kh} - E \right] P_{2M} e^{-\alpha R}$$

$$+ \sqrt{8} P_{2M+3} P_{2M+4} \frac{e^{-kh/P} 2^{M+4}}{kh} P_{2M+1} e^{-\alpha R} = 0 \quad (\ell=2; k=M) \rightarrow (K=2M) \quad (6.22b)$$

These equations (6.20) to (6.22) are designated

$$f_K = 0 \quad K = 1, 2, \dots, 2M$$

The normalization condition provides the equation

$$f_{2M+1} = P_{2M-1}^2 + P_{2M}^2 - 1 = 0 \quad (6.23)$$

The integrals are evaluated by first separating the integral on  $[0, \infty]$  as

$$\int_0^{\infty} F(r) dr = \int_0^R F(r) dr + \int_R^{\infty} F(r) dr$$

and evaluating the integral on  $[0, R]$  by the trapezoidal rule

$$\int_0^R F(r) dr = h \sum_{k=1}^{M-1} F(kh) + \frac{h}{2} [F(0) + F(R)]$$

and the integral on  $[R, \infty]$  analytically with the asymptotic forms of the radial functions. The effective range equation is labelled  $f_{2M+2}$ .

$$\int_0^{\infty} [e^{-2\alpha r} - (u_1^2 + u_2^2)] dr = \frac{\rho}{2}$$

$$h \sum_{k=1}^{M-1} \left[ e^{-2\alpha k h} - (P_{1k}^2 + P_{2k}^2) \right] + \frac{h}{2} [1 + e^{-2\alpha R} (1 - P_{2M-1}^2 - P_{2M}^2)] + \int_R^{\infty} e^{-2\alpha r} (1 - P_{2M-1}^2 - P_{2M}^2) dr$$

$$= \frac{\rho}{2} \text{ gives}$$

$$f_{2M+2} = \sum_{k=1}^{M-1} e^{-2\alpha k h} - \sum_{k=1}^{M-1} (P_{1k}^2 + P_{2k}^2) + \frac{1}{2} - \frac{e^{-2\alpha R} (P_{2M-1}^2 + P_{2M}^2 - 1)}{2} \left( 1 + \frac{1}{\alpha h} \right) - \frac{\rho}{2h} = 0 \quad (6.24)$$

$$\text{using } \int_R^{\infty} e^{-2\alpha r} dr = \left[ \frac{e^{-2\alpha r}}{-2\alpha} \right]_R^{\infty} = \frac{e^{-2\alpha R}}{2\alpha}$$

Next is the % D-state equation

$$\int_0^{\infty} u_2^2 dr = P_D \int_0^{\infty} (u_1^2 + u_2^2) dr$$

which, in terms of the elements of the vector of unknowns  $\vec{P}$ , is

$$h \sum_{k=1}^{M-1} P_{2k}^2 + \frac{h}{2} P_{2M}^2 e^{-2\alpha R} + P_{2M}^2 \int_R^{\infty} e^{-2\alpha r} dr - P_D \left[ \sum_{k=1}^{M-1} (P_{1k}^2 + P_{2k}^2) + \frac{h}{2} (P_{2M-1}^2 + P_{2M}^2) e^{-2\alpha R} - (P_{2M-1}^2 + P_{2M}^2) \int_R^{\infty} e^{-2\alpha r} dr \right] = 0$$

so

$$f_{2M+3} = (1 - P_D) \sum_{k=1}^{M-1} P_{2k}^2 - P_D \sum_{k=1}^{M-1} P_{1k}^2 + (1 - P_D) P_{2M}^2 \frac{e^{-2\alpha R}}{2} \left( 1 + \frac{1}{\alpha h} \right) - P_D P_{2M-1}^2 \frac{e^{-2\alpha R}}{2} \left( 1 + \frac{1}{\alpha h} \right) = 0 \quad (6.25)$$

The final equation comes from fitting the quadrupole moment  $Q$  in

$$\frac{\sqrt{2}}{10} \int_0^{\infty} (u_1 u_2 - \frac{1}{2\sqrt{2}} u_2^2) r^2 dr - Q \int_0^{\infty} (u_1^2 + u_2^2) dr = 0$$

In finite difference form on  $[0, R]$  and with the exponential form

beyond  $R$ , this gives

$$\frac{\sqrt{2}}{10} \left[ h \sum_{k=1}^{M-1} P_{1k} P_{2k} k^2 h^2 + \frac{h}{2} P_{2M} P_{2M-1} R^2 e^{-2\alpha R} - \frac{h}{2\sqrt{2}} \sum_{k=1}^{M-1} P_{2k}^2 k^2 h^2 - \frac{h}{4\sqrt{2}} P_{2M}^2 R^2 e^{-2\alpha R} \right]$$

$$+P_{2M}P_{2M-1} \int_R^\infty e^{-2\alpha r} r^2 dr - \frac{P_{2M}^2}{2\sqrt{2}} \int_R^\infty e^{-2\alpha r} r^2 dr \left] - Q \left[ h \sum_{k=1}^{M-1} (P_{1k}^2 + P_{2k}^2) + \frac{h}{2} e^{-2\alpha R} (P_{2M-1}^2 + P_{2M}^2) + (P_{2M-1}^2 + P_{2M}^2) \int_R^\infty e^{-2\alpha r} dr \right] = 0$$

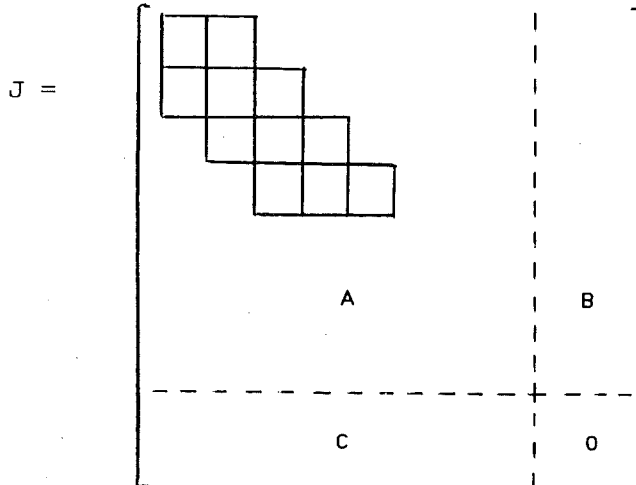
Using  $\int_R^\infty e^{-2\alpha r} r^2 dr = e^{-2\alpha R} \left( \frac{R^2}{2\alpha} + \frac{R}{2\alpha^2} + \frac{1}{4\alpha^3} \right)$  we get

$$\frac{\sqrt{2}}{10} \sum_{k=1}^{M-1} P_{1k} P_{2k} k^2 h^2 - \frac{1}{20} \sum_{k=1}^{M-1} P_{2k}^2 k^2 h^2 + \frac{\sqrt{2}}{10} P_{2M} P_{2M-1} e^{-2\alpha R} \left( \frac{R^2}{2} \left\{ 1 + \frac{1}{\alpha h} \right\} + \frac{R}{2\alpha^2 h} + \frac{1}{4\alpha^3 h} \right) - \frac{1}{20} P_{2M}^2 e^{-2\alpha R} \left( \frac{R^2}{2} \left\{ 1 + \frac{1}{h} \right\} + \frac{R}{2\alpha^2 h} + \frac{1}{4\alpha^3 h} \right) - Q \sum_{k=1}^{M-1} (P_{1k}^2 + P_{2k}^2) - Q (P_{2M-1}^2 + P_{2M}^2) \cdot \frac{e^{-2\alpha R}}{2} \left( 1 + \frac{1}{\alpha h} \right) = 0 = f_{2M+4}$$

The system of equations is solved by the generalized Newton-Raphson method used in the previous chapter with a Jacobian matrix

$$J_{kk'} = \frac{\partial f_k}{\partial P_{k'}}$$

of the form



where A is a (2M×2M) block tridiagonal matrix with (2×2) matrices on the diagonal and adjacent to the diagonal, B is a (2M×4) matrix and C a (4×2M) matrix. The matrix elements of the Jacobian matrix are given in Appendix 3.

### 6.3 Results and conclusions

The normalization and potential parameters and the deuteron radial wavefunctions were calculated for  $R = 10, 15$  and  $20$  fm. For each of these Hulthén wavefunctions [47] defined in terms of the variable  $x = \alpha r$ ,

$$u_1(x) = N_1 (1 - e^{-\beta x}) e^{-x} \quad (6.27a)$$

$$u_2(x) = N_2 (1 - e^{-\gamma x})^2 e^{-x} \left[ 1 + \frac{3(1 - e^{-\gamma x})}{x} + \frac{3(1 - e^{-\gamma x})^2}{x^2} \right] \quad (6.27b)$$

were used as starting approximations, with  $\beta = 4.637$  and  $\gamma = 2.936$ .

Initial values of 0.9 and 0.02 were chosen for  $N_1$  and  $N_2$  and the potential parameters were taken from a soft-core triplet-even potential calculated by Gammel, Christian and Thaler [34] which corresponded to a % D state value of 3.57. Of the data to which we fit the potential, the % D state value contains the greatest uncertainty; in the calculation we took a value of 3.9%.

The calculated wavefunctions for different values of  $R$  are shown in Figures 16 - 21. The calculated normalization parameters are used to give the asymptotic forms of the radial wavefunctions and these are also shown. It can be seen that the S-wavefunctions rapidly approach their asymptotic limits for all values of  $R$ , while the D-wavefunctions do not assume the exponential form until  $R$  is nearly reached. In Figure 22 we show that the S-wavefunctions are not greatly affected by changes in  $R$  and that the solutions we have obtained differ only slightly from the Hulthén S-wavefunction. A greater difference is apparent in the D-wavefunctions given in Figure 23. The values calculated for the normalization and potential parameters are listed in Table 7 and the

potentials for  $R = 10$  fm and  $R = 20$  fm shown in Figures 24 - 27.

TABLE 7					
Normalization parameters		Central potential		Tensor force	
S	D	$V_C$	$r_C$	$V_t$	$r_t$
$R = 10$ fm					
$9.97 \times 10^{-1}$	$7.17 \times 10^{-2}$	-11.88	1.87	-76.72	1.09
$R = 15$ fm					
$9.99 \times 10^{-1}$	$5.29 \times 10^{-2}$	-14.35	1.74	-68.96	1.14
$R = 20$ fm					
$9.99 \times 10^{-1}$	$4.38 \times 10^{-2}$	-14.49	1.73	-68.31	1.14

FIGURE 16

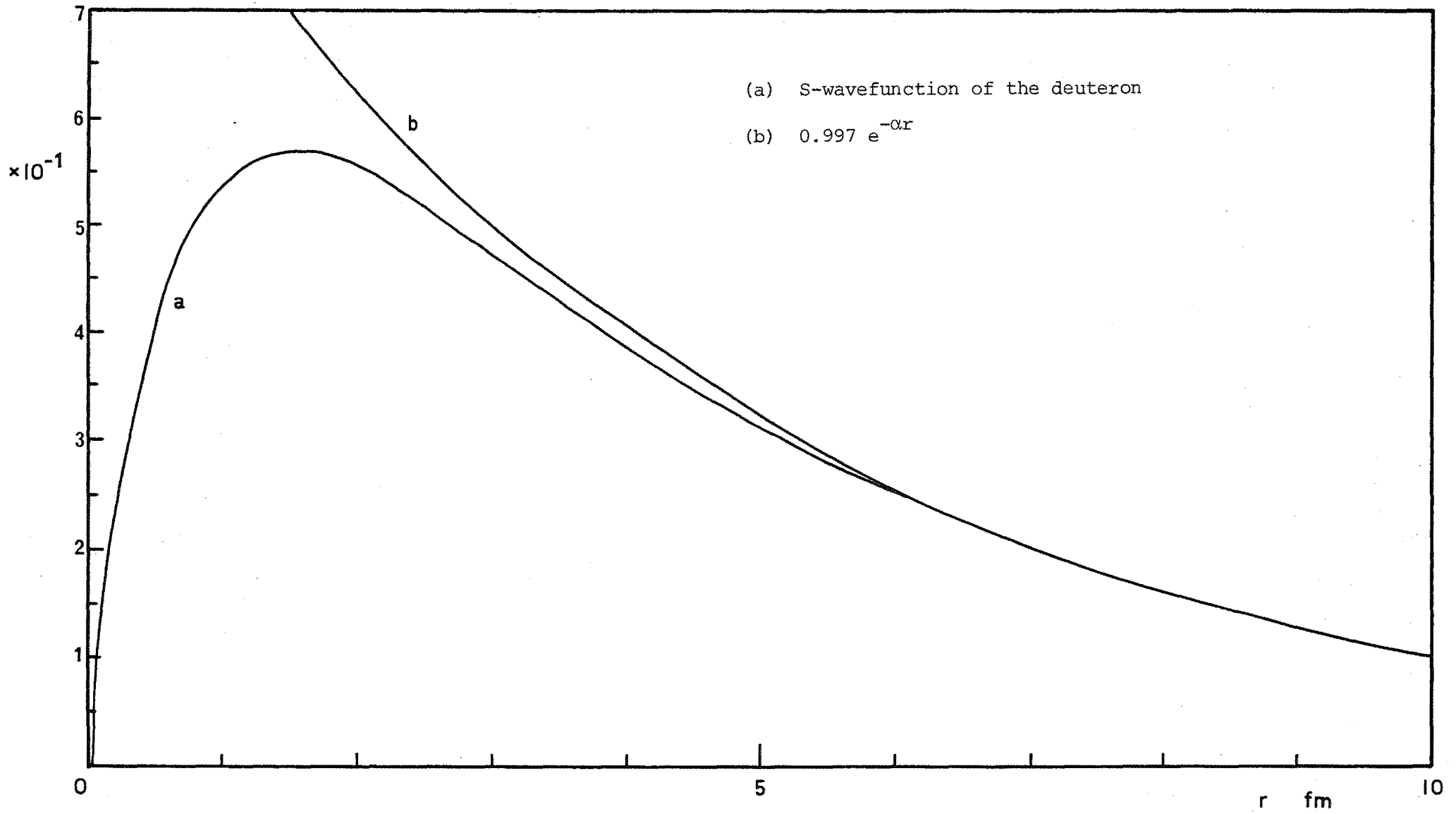


FIGURE 17

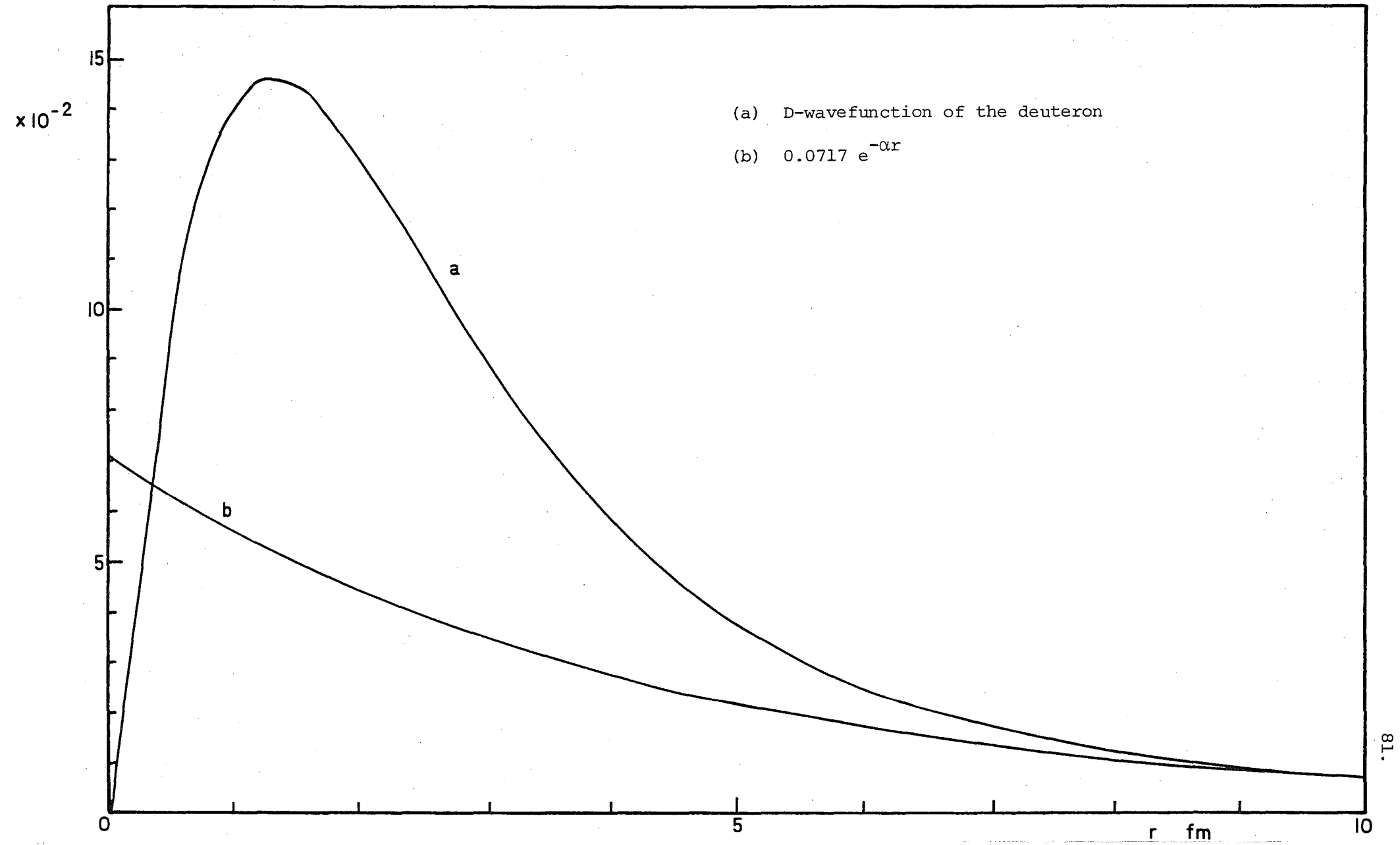




FIGURE 18

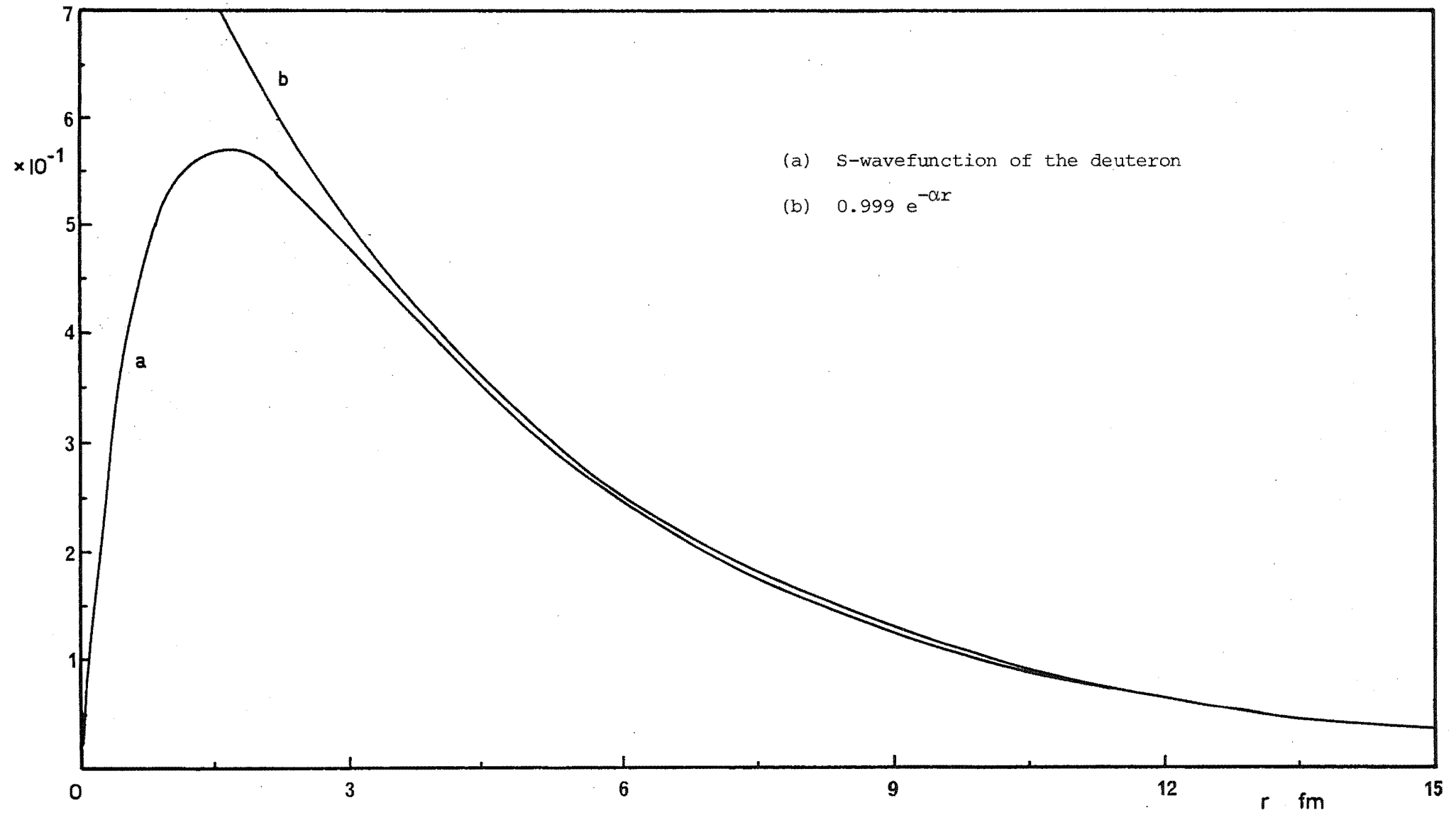


FIGURE 19

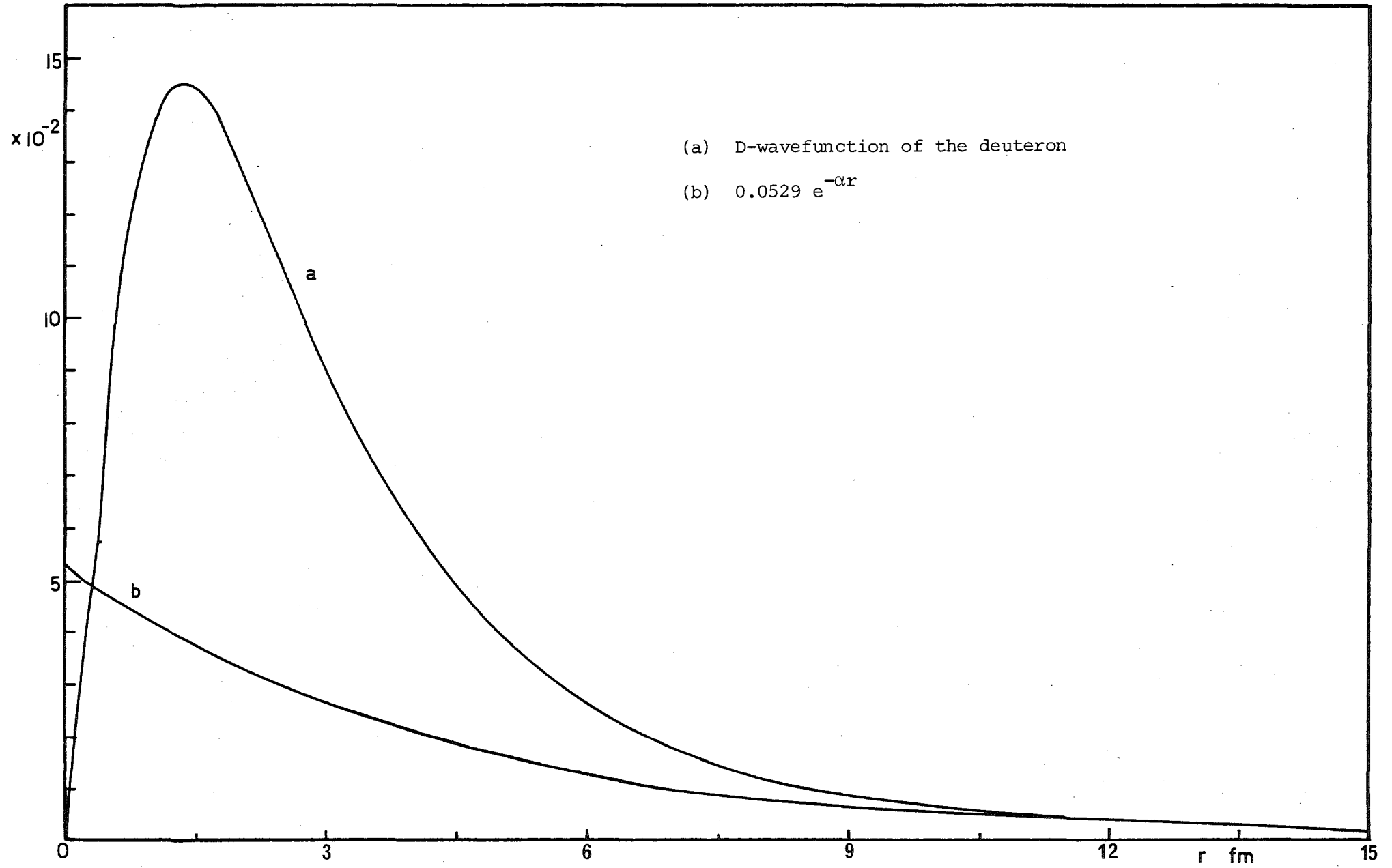


FIGURE 20

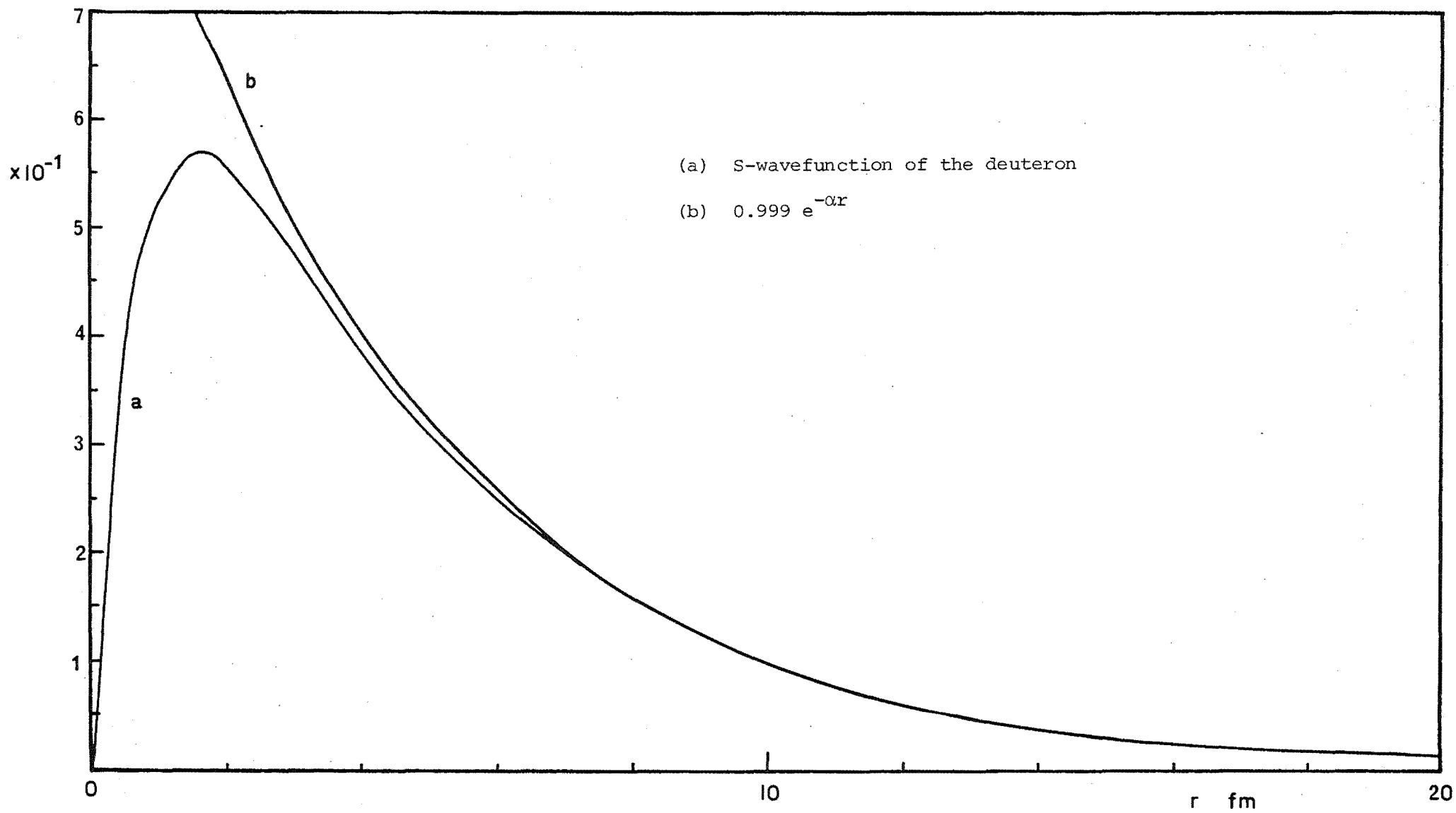


FIGURE 21

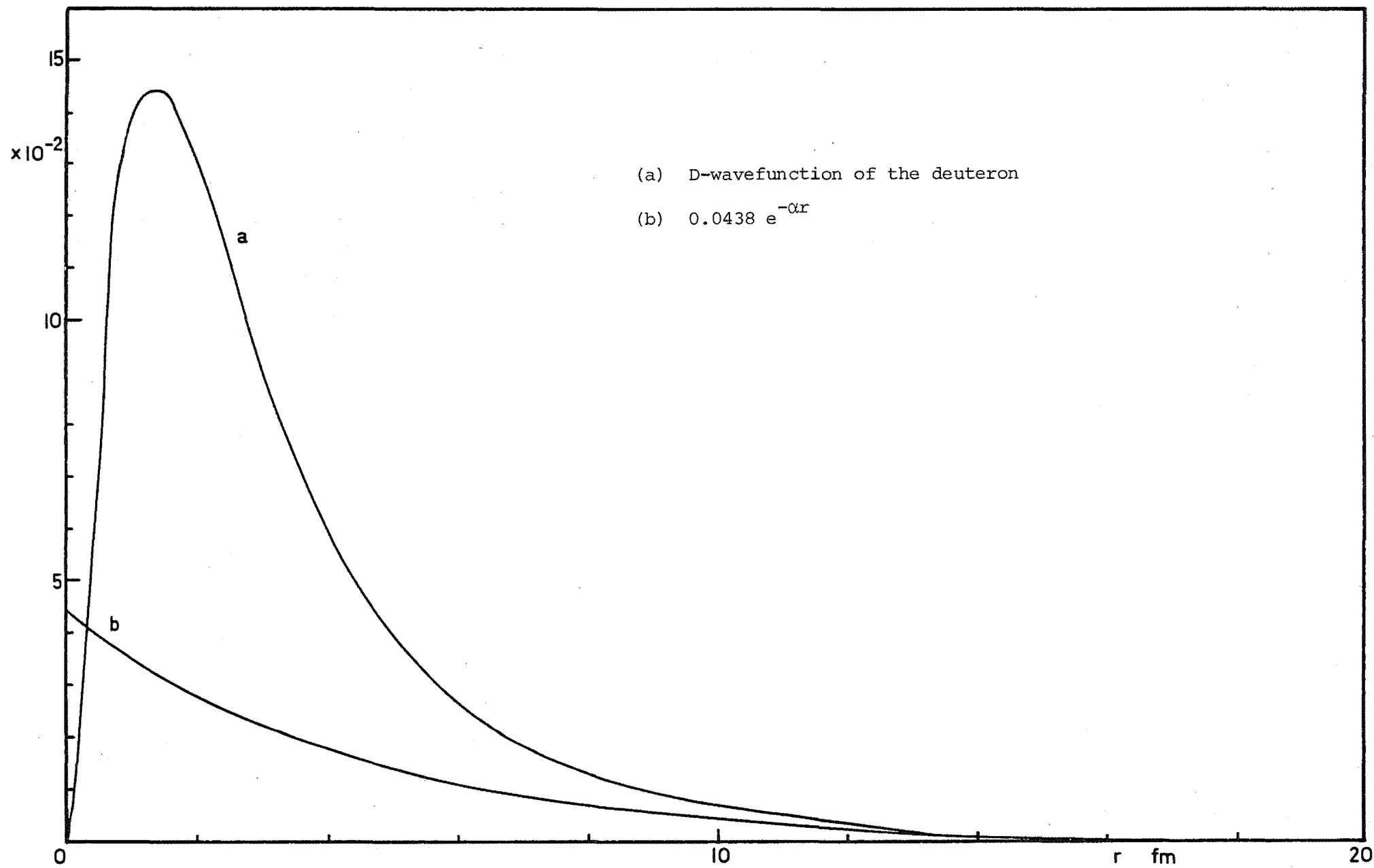
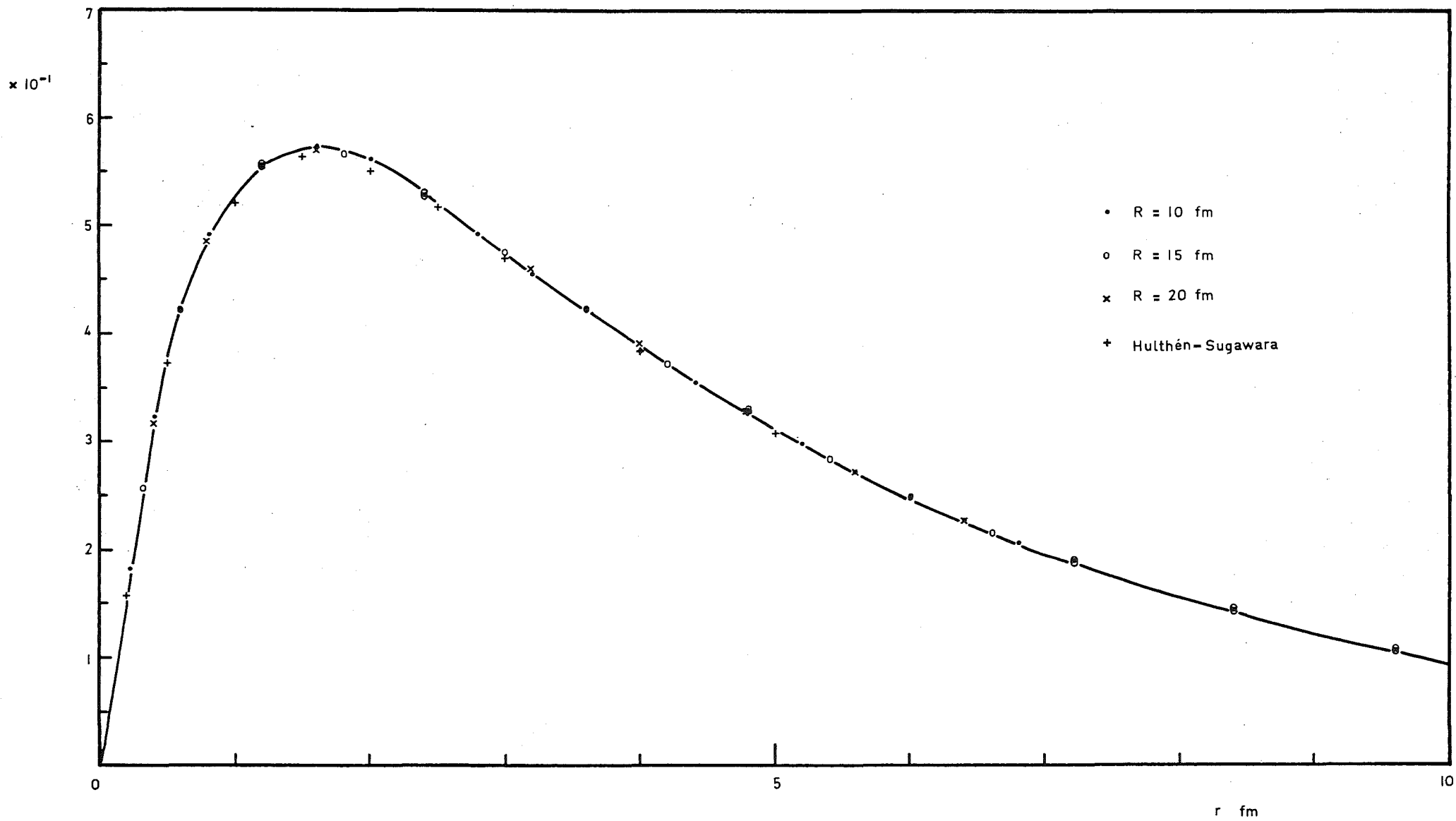


FIGURE 22

S-Wavefunctions of the deuteron.



D-wavefunctions of the deuteron

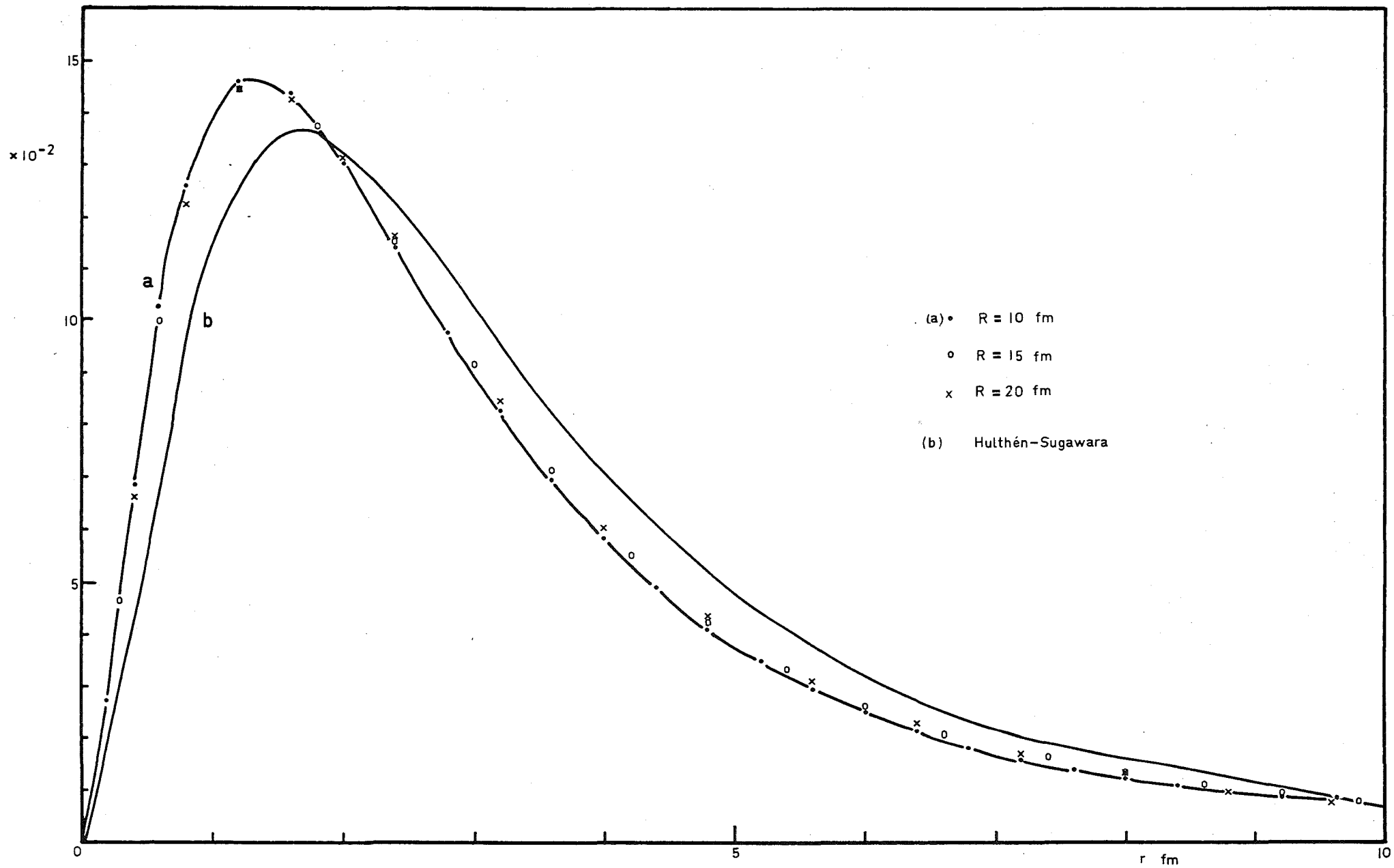
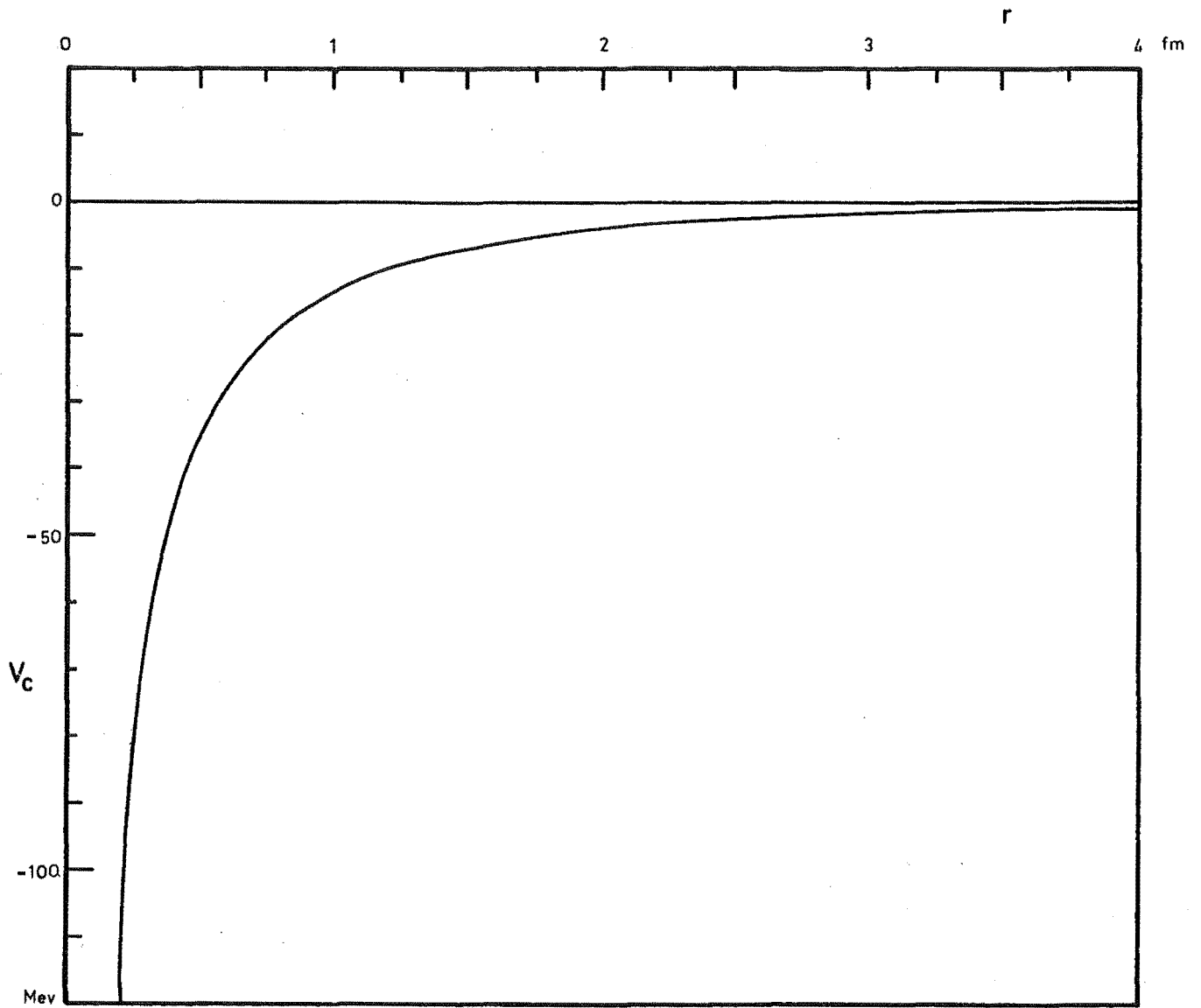
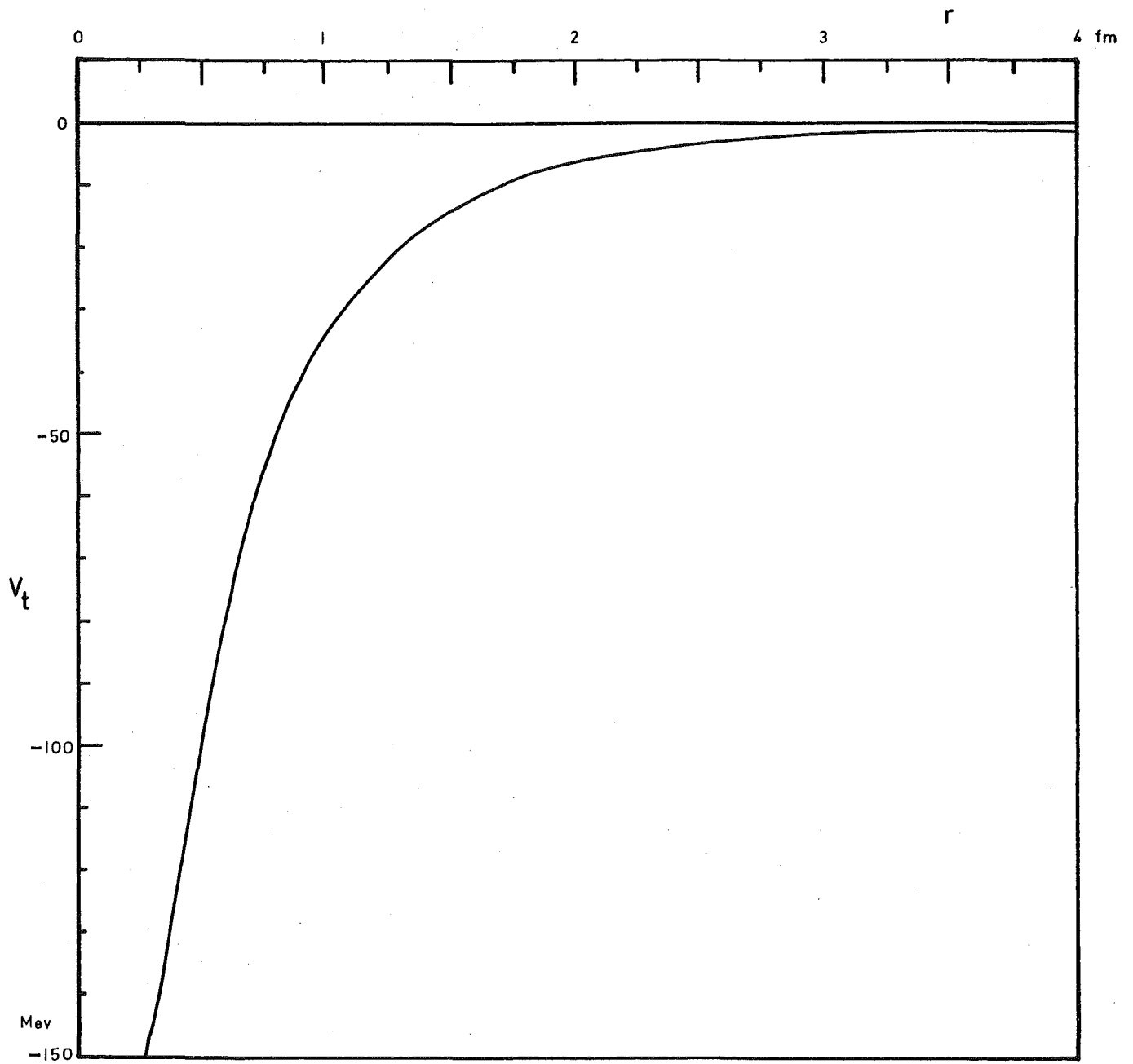


FIGURE 24



Central potential calculated with  $R = 10$  fm

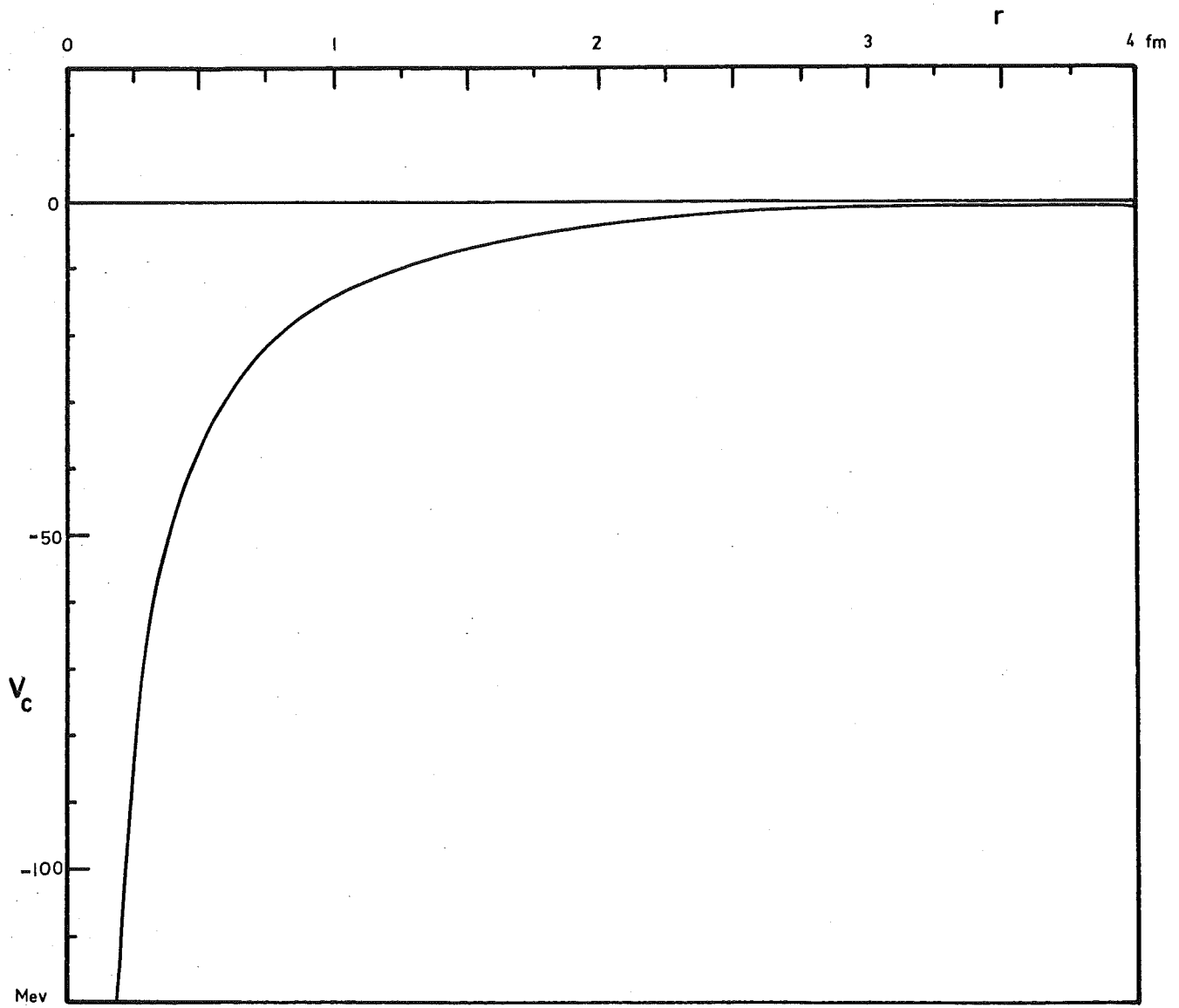
FIGURE 25



Tensor potential calculated with  $R = 10$  fm

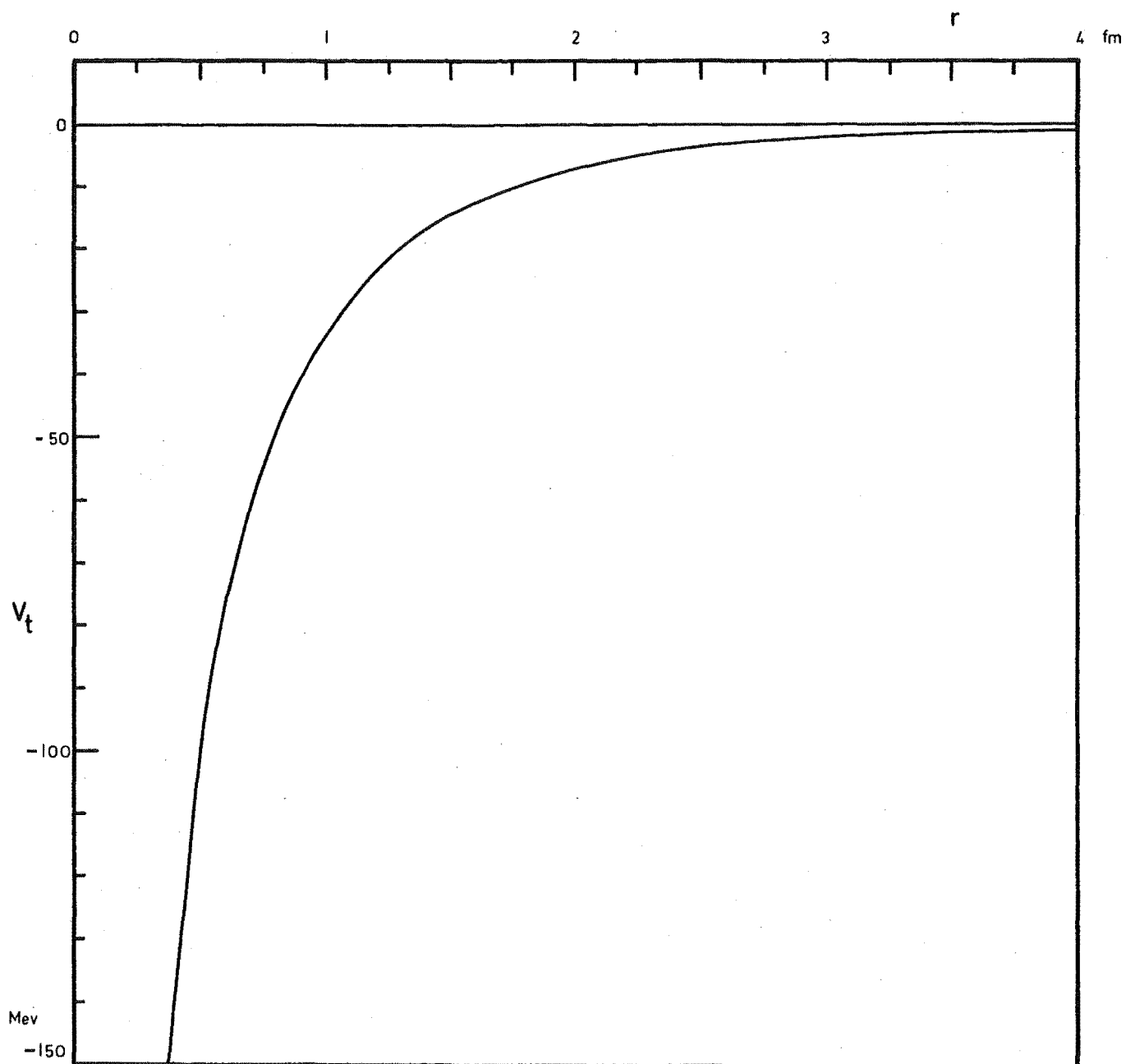


FIGURE 26



Central potential calculated with  $R = 20$  fm

FIGURE 27



Tensor potential calculated with  $R = 20$  fm.

As the value of  $R$  is increased the potential parameters vary more slowly but cannot be determined without obtaining one of the parameters by an independent calculation. Because of the normalization chosen (6.13) the upper end-point is floating. If we let  $R \rightarrow \infty$  we cannot impose the condition the radial functions tend to zero exponentially and the effective range equation cannot be used. It would seem however that  $R$  should be chosen to be large since the depth of the central part of the potential is too small otherwise. The distance at which the wavefunctions tend to their asymptotic forms has been discussed by Biedenharn, Blatt and Kalos [48] and is found to be greater than the "deuteron radius", 4.316 fm.

The present state of the low-energy two-nucleon data is such that potentials cannot be calculated to any great degree of accuracy. We have given here a method which can in principle calculate the wavefunctions and potential parameters accurately but, as we have discussed in Section 6.1, some of the constants introduced in our constraints are not very well determined. There is also the problem matching the close-separation wavefunctions with their asymptotic forms; we could resolve this if an additional constraint, such as the average neutron-proton distance in the deuteron, were known. We have however obtained potentials consistent with the known two-body data and the calculated wavefunctions are of the correct magnitude and shape for deuteron wavefunctions.

#### SUMMARY AND CONCLUSIONS

In this thesis we have examined some of the problems encountered in nuclear structure theory. The two main problems in which we are interested are (i) the calculation of a wavefunction which approximates closely an eigenfunction of a given Hamiltonian, and (ii) the calculation

of a nuclear potential fitted to the low-energy neutron-proton data. For the first of these the choice of a Hamiltonian with hard-core internucleon potentials necessitated the use of effective interactions derived from the original ones by a unitary transformation. This led to a relationship with the correlated wavefunction method which was exact only in the two-nucleon case. Neglect of the many-body terms involving more than two nucleons meant that the parameter introduced by the unitary transformation, or, equivalently, the parameter contained in the correlation function, could not be obtained variationally. With the effective Hamiltonian  $H = T + V(\beta)$  the approximate wavefunction is implicitly dependent on the transformation parameter. It has been previously suggested by Slater [32] that the virial theorem can be used to improve approximate wavefunctions in that it provides an independent and sensitive check on the wavefunction through the relation between the kinetic and potential energies. Applying this theorem with a suitable choice of the radial transformation generating the velocity dependent potentials, we have obtained results for nuclear matter comparable with those obtained by the Brueckner theory.

In applying the general procedure to finite nuclei, we have made use of the fact that the intrinsic nuclear energy is expressible in terms of two-particle matrix elements. Again we have taken a transformation which is exact only in the two-particle case but this time we have made it nucleon number-dependent. The transformation of the two-particle wavefunctions from single-particle to relative and center-of-mass coordinates is simply a change of representation and must therefore be unitary. We can carry out the inverse transformation

$$|N, n\sigma\rangle = \sum_{\alpha\beta} |\alpha\beta\rangle \langle \alpha\beta | N, n\sigma\rangle$$

where the  $\langle \alpha\beta | N, n\sigma \rangle$  are the transformation coefficients and are not functions of the coordinates. If the left hand side of the above equation is multiplied by a correlation function  $C$  depending on the relative coordinate, as we would need to have to maintain the equality of the two-particle matrix elements of the effective and realistic Hamiltonians (see eqn (4.13)), the problem of expressing the relative and centre of mass wavefunction in terms of single-particle functions becomes considerably more difficult unless  $C$  has a simple expression in terms of the single-particle coordinates. For a correlation function appropriate to hard-core interactions we cannot express  $C$  in these coordinates and even for a well-behaved  $C$  it is much easier to work with the effective Hamiltonian and simple trial functions. A point which we note here is that the equivalence of the total energy (through the two-particle matrix elements) means that when the Hamiltonian is chosen so that the effective interaction corresponds to a well-behaved correlation function, the effective interaction with simple trial wavefunctions, e.g. eigenfunctions of the single-particle orbital angular momentum, is equivalent to a description, with the realistic Hamiltonian, in which there is a mixing of angular states since  $C$  can be expressed in a Legendre expansion

$$C(r) = \sum_{\lambda=0}^{\infty} C_{\lambda}(r_1, r_2) \frac{4\pi}{2\lambda+1} \sum_{\mu=-\lambda}^{+\lambda} Y_{\lambda}^{\mu*}(\theta_1, \phi_1) Y_{\lambda}^{\mu}(\theta_2, \phi_2)$$

This also applies to hard-core interactions if we separate the purely hard-core and the correlating effects of  $C$  by separating  $C$  as a product of a step function and a well-behaved function of the relative coordinate.

We have shown how the effective interaction-correlation function approach, which is essential for hard-core potentials, can lead to simpler trial wavefunctions in a many-body system. This has encouraged

the use of rather crude trial wavefunctions since compensating changes in the total wavefunction may be introduced as "correlation". This has been shown in our soft-core potential calculations, in which we have calculated the radial functions of the  $\text{He}^4$  nucleus to a greater accuracy than could be obtained by Gaussian radial wavefunctions. The calculated energy was comparable with that obtained in second-or~~th~~third-order correlation by Fantoni et al [44] and a more accurate evaluation would require a correlation function or higher configurations.

The finite-difference method lends itself to potential calculations since potentials cannot be fitted accurately unless the wavefunctions can be calculated accurately. Although the low-energy neutron-proton data is insufficient to determine the two-nucleon potential, we have presented in Chapter 6 a method for calculating potentials. The advantage of this method is that the potential parameters are treated in the same manner as the unknown wavefunction points and consequently the systematic fitting to the neutron-proton data could be carried out within the Newton-Raphson iteration which calculated all the unknowns. This avoided the need to guess some of the parameters and fit the remainder to the data, since the equations giving the  $\%$ -D state, quadrupole moment and effective range were included in our system of simultaneous equations. However, the choice of normalization and the fact that we did not know the distance,  $R$ , at which the radial functions approached their asymptotic form meant that we could not uniquely determine the neutron-proton potential. The rapid convergence of the Newton-Raphson iteration makes it a simple matter to calculate potentials for a range of values of  $R$  and the potential could be determined if the resulting wavefunctions were used to calculate a further known property of the neutron-proton system.

To improve upon the methods used in our calculations on finite nuclei we could use the effective Hamiltonian in a finite difference calculation. This would allow a more accurate determination of the single-particle wavefunctions and the results should not be so sensitive to the choice of transformation generating the two-particle correlation functions. In choosing a functional form for the transformed radial variable an arbitrary restriction is imposed on the system, but its effect will be lessened if the correlation functions become less important. Alternatively, simple radial functions which transform readily to relative and pair centre of mass coordinates may be assumed and the pair correlation function determined numerically. However more accurate calculations would require better-determined potentials which not only fit the two-nucleon data but are also sufficiently well-behaved to use in many-nucleon calculations. It is uncertain whether the two-nucleon interaction is representable by a potential, but for the purposes of nuclear structure calculations it is considered sufficient to approximate the interaction with a potential. While such uncertainties remain we cannot hope to achieve results comparable in accuracy with those obtainable in atomic structure calculations and further work needs to be done on the many-body aspect and the two-nucleon interaction for nuclear systems before good results can be obtained from ab initio calculations.

APPENDIX 1A

A. Direct integrals for nuclear matter calculations.

The general expression for the direct integral is

$$\frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} e^{i\vec{k}\cdot\vec{r}} w e^{-i\vec{k}\cdot\vec{r}} \quad (1)$$

For each charge-spin state  $\alpha$ , the interaction is of the form

$$\begin{aligned} w = & \frac{1}{2} \left\{ (B^2 - 1 - g) P_r^2 + P_r^2 (B^2 - 1 - g) \right\} + \frac{1}{2} (g p^2 + p^2 g) + \frac{B}{2} \frac{\partial^2 B}{\partial r^2} + \\ & + \frac{3}{4} \left( \frac{\partial B}{\partial r} \right)^2 + V_c(\tilde{r}) \equiv \frac{1}{2} (V_2(r) P_r^2 + P_r^2 V_2(r)) + \\ & + \frac{1}{2} (V_3(r) p^2 + p^2 V_3(r)) + V_0(r) \end{aligned} \quad (2)$$

For  $V_0(r)$ , equation (1) simplifies to

$$\begin{aligned} & \frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} V_0(r) \\ & = \frac{(4\pi)^2}{(2\pi)^3} \left[ \frac{k^3}{3} - \frac{3k^4}{8k_F} + \frac{k^6}{12k_F^3} \right]_0^{k_F} \int_0^\infty r^2 dr V_0(r) \\ & = \frac{k_F^3}{12\pi} \int_0^\infty V_0(r) r^2 dr \end{aligned} \quad (3)$$

To obtain the contribution from the term containing  $V_2(r)$  we use

$$P_r^2 = - \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right)$$

$$\begin{aligned} \text{Then } & \frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} e^{i\vec{k}\cdot\vec{r}} V_2(r) P_r^2 e^{-i\vec{k}\cdot\vec{r}} \\ & = \frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} e^{i\vec{k}\cdot\vec{r}} V_2(r) \\ & \quad \left[ - \left( \frac{-i\vec{k}\cdot\vec{r}}{r} \right)^2 - \frac{2}{r} \left( \frac{-i\vec{k}\cdot\vec{r}}{r} \right) \right] e^{-i\vec{k}\cdot\vec{r}} \end{aligned}$$



$$= \frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} \left( \frac{\vec{k} \cdot \vec{r}}{r} \right)^2 V_2(r)$$

$$+ \frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} \left( \frac{i\vec{k} \cdot \vec{r}}{r} \right) V_1(r)$$

where  $V_1(r) = \frac{2}{r} V_2(r)$  (4)

Since  $p_r^2$  is hermitian

$$\int d\vec{r} e^{i\vec{k} \cdot \vec{r}} p_r^2 V_2(r) e^{-i\vec{k} \cdot \vec{r}} = \int d\vec{r} \left( \frac{\vec{k} \cdot \vec{r}}{r} \right)^2 V_2(r) - \int d\vec{r} \left( \frac{i\vec{k} \cdot \vec{r}}{r} \right) V_2(r)$$

so

$$\frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} e^{i\vec{k} \cdot \vec{r}} \frac{1}{2} (V_2 p_r^2 + p_r^2 V_2) e^{-i\vec{k} \cdot \vec{r}}$$

$$= \frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} \left( \frac{\vec{k} \cdot \vec{r}}{r} \right)^2 V_2(r)$$

$$= \frac{1}{(2\pi)^3} \int_0^{k_F} k^2 dk \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int_0^\infty r^2 dr V_2(r) \int d\hat{k} \int d\hat{r} \left( \frac{\vec{k} \cdot \vec{r}}{r} \right)^2 \quad (5)$$

$$\int d\hat{k} \int d\hat{r} \left( \frac{\vec{k} \cdot \vec{r}}{r} \right)^2 = k^2 \int d\hat{k} \int d\hat{r} \cos^2 \theta \quad \text{where } \theta = \cos^{-1} \left( \frac{\vec{k} \cdot \vec{r}}{kr} \right)$$

$$= \frac{(4\pi)^2}{3} k^2$$

Substituting this in (5) and integrating over k we get

$$\frac{2}{3\pi} \left[ \frac{k^5}{5} - \frac{3k^6}{12k_F} + \frac{k^8}{16k_F^3} \right]_0^{k_F} \int_0^\infty r^2 dr V_2(r)$$

$$= \frac{k_F^5}{120\pi} \int_0^\infty V_2(r) r^2 dr \quad (6)$$

In a similar manner, but using

$$p^2 e^{-i\vec{k} \cdot \vec{r}} = k^2 e^{-i\vec{k} \cdot \vec{r}}$$

we obtain for the remaining direct integral

$$\frac{1}{(2\pi)^3} \int d\vec{k} k^2 \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} V_3(r)$$

$$= \frac{k_F^5}{40\pi} \int_0^{\infty} V_3(r) r^2 dr \quad (7)$$

The direct integrals for calculating the virial are obtained using the same expressions but with a redefinition of the radial parts  $V_0$ ,  $V_2$  and  $V_3$ .

## APPENDIX 1B

B. Exchange integrals for nuclear matter calculations

The functions  $V_0$ ,  $V_1$ ,  $V_2$  and  $V_3$  are those already used in Part A of this appendix. For  $V_0(r)$  we now have the integral

$$\frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} V_0(r) e^{-2i\vec{k}\cdot\vec{r}} \quad (8)$$

Expanding  $e^{-2i\vec{k}\cdot\vec{r}}$  as

$$4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (-i)^{\ell} j_{\ell}(2kr) Y_{\ell}^{m*}(\hat{k}) Y_{\ell}^m(\hat{r}) \quad (9)$$

and substituting in (8) gives, after carrying out the angular integrations,

$$\frac{2}{\pi} \int_0^{\infty} r^2 dr V_0(r) \int_0^{k_F} k^2 dk \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) j_0(2kr)$$

In terms of the variables  $y = 2kr$ ,  $z = 2k_F r$ , the  $k$ -integration may be written as

$$\int_0^{k_F} k^2 dk \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) j_0(2kr) = \frac{k_F^3}{z^3} \int_0^z \left( y - \frac{3y^3}{2z} + \frac{y^5}{2z^3} \right) j_0(y) dy$$

and a function  $k_0(z)$  is defined by

$$k_0(z) = \frac{1}{z^3} \int_0^z \left( y - \frac{3y^3}{2z} + \frac{y^5}{2z^3} \right) j_0(y) dy \quad (10)$$

$$\text{and } k_0(z) = \frac{3}{z^6} (z^2 \cos z - 4 \cos z - 4z \sin z + z^2 + 4) \quad (11)$$

For small values of the argument the expansion

$$k_0(z) = 3 \sum_{n=0}^{\infty} (-1)^n z^{2n} \frac{(2n+5)(2n+2)}{(2n+6)!} \quad (12)$$

was used, and

$$\lim_{z \rightarrow 0} k_0(z) = \frac{1}{24} \quad (13)$$

Then we obtain for (8)

$$\frac{2k_F^3}{\pi} \int_0^\infty V_0(r) k_0(2k_F r) r^2 dr \quad (14)$$

In the exchange term the integrals containing  $V_1(r)$  no longer vanish; instead we have

$$\frac{-1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} \left( \frac{-i\vec{k} \cdot \vec{r}}{r} \right) V_1(r) e^{-2i\vec{k} \cdot \vec{r}} \quad (15)$$

Since

$$\frac{i\vec{k} \cdot \vec{r}}{r} = ik \cos \theta = \frac{4\pi}{3} \sum_{m=-1}^{+1} Y_1^{m*}(\hat{k}) Y_1^m(\hat{r})$$

the angular integrations give

$$\begin{aligned} \int d\hat{k} \int d\hat{r} \left( \frac{i\vec{k} \cdot \vec{r}}{r} \right) e^{-2i\vec{k} \cdot \vec{r}} &= -ik \frac{(4\pi)^2}{3} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{m'=-1}^1 (-i)^\ell j_\ell(2kr) \delta_{\ell 1} \delta_{mm'} \\ &= - (4\pi)^2 j_1(2kr) k \end{aligned}$$

so (15) becomes

$$\begin{aligned} &\frac{2}{\pi} \int_0^{k_F} k^3 dk \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int_0^\infty r^2 dr V_1(r) j_1(2kr) \\ &= \frac{2}{\pi} \int_0^\infty r^2 dr V_1(r) \int_0^{k_F} dk \left( k^3 - \frac{3k^4}{2k_F} + \frac{k^6}{2k_F^3} \right) j_1(2kr) \\ &= \frac{2k_F^4}{\pi} \int_0^\infty V_1(r) k_1(2k_F r) r^2 dr \quad (16) \end{aligned}$$

where

$$k_1(z) = \frac{1}{z^4} \int_0^{k_F} \left( y^3 - \frac{3y^4}{2z} + \frac{y^6}{2z^3} \right) j_1(y) dy \quad (17)$$

$$= \frac{3}{z^7} (8z^2 \cos z - 24 \cos z + z^3 \sin z - 24z \sin z + 4z^2 + 24)$$

for which  $\lim_{z \rightarrow 0} k_1(z) = 0$  (18)

and  $\lim_{z \rightarrow 0} \frac{1}{z} k_1(z) = \frac{1}{240}$  (19)

The series expansion for  $k_1$  is

$$k_1(z) = 3 \sum_{n=0}^{\infty} (-1)^{n+1} z^{2n-1} \frac{(2n+5)(2n+2)2n}{(2n+6)!} \quad (20)$$

The exchange integrals involving  $V_2(r)$  are

$$\frac{1}{(2\pi)^3} \int d\vec{k} \left( 1 - \frac{3k}{2k_F} + \frac{k^3}{2k_F^3} \right) \int d\vec{r} \left( \frac{\vec{k} \cdot \vec{r}}{r} \right)^2 V_2(r) e^{-2i\vec{k} \cdot \vec{r}} \quad (21)$$

With

$$\left( \frac{\vec{k} \cdot \vec{r}}{r} \right)^2 = k^2 \cos^2 \theta = k^2 \left( \frac{8\pi}{15} \sum_{m=-2}^{+2} Y_2^{m*}(\hat{k}) Y_2^m(\hat{r}) + \frac{4\pi}{3} \right)$$

the angular integrations give

$$k^2 \left( \frac{32\pi^2}{15} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{m'=-2}^{+2} (-i)^{\ell} j_{\ell}(2kr) \delta_{\ell 2} \delta_{mm'} + \frac{(4\pi)^2}{3} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (-i)^{\ell} j_{\ell}(2kr) \delta_{\ell 0} \delta_{m0} \right)$$

$$= k^2 (4\pi)^2 \left( \frac{1}{3} j_0(2kr) - \frac{2}{3} j_2(2kr) \right)$$

This leads to two  $k$ -integrations, the first, containing  $j_0$ , is

$$\frac{1}{z^5} \int_0^z \left( y^4 \frac{3y^5}{2z} + \frac{y^7}{2z^3} \right) dy = k_3(z) \quad (22)$$

$k_3$  is obtained in a similar way to  $k_0$  giving

$$k_3(z) = \frac{3}{z^8} (z^4 \cos z - 48z^2 \cos z + 120 \cos z - 10z^3 \sin z + 120z \sin z - 12z^2 - 120) \quad (23)$$

and

$$\lim_{z \rightarrow 0} k_3(z) = \frac{1}{80} \quad (24)$$

$$\text{Also } k_3(z) = 3 \sum_{n=0}^{\infty} (-1)^n z^{2n} \frac{(2n+7)(2n+4)(2n+3)(2n+2)}{(2n+8)!} \quad (25)$$

The other  $k$ -integration involves  $j_2$  and can be written as

$$\frac{1}{z^5} \int_0^z \left( y^4 \frac{3y^5}{2z} + \frac{y^7}{2z^3} \right) j_2(y) dy \equiv k_2'(z) \quad (26)$$

Using the property of the spherical Bessel functions that

$$j_2(y) = \frac{3}{y} j_1(y) - j_0(y) \quad (27)$$

we obtain, by comparison with equations (17) and (22),

$$k_2'(z) = \frac{3k_1(z)}{z} - k_3(z) \quad (28)$$

$$\begin{aligned} \text{Defining } k_2(z) &\equiv \frac{k_3(z)}{3} - \frac{2}{3} \left[ \frac{3k_1(z)}{z} - k_3(z) \right] \\ &= k_3(z) - \frac{2k_1(z)}{3} \end{aligned} \quad (29)$$

We obtain for the integral (14)

$$\frac{2k_F^5}{\pi} \int_0^{\infty} V_2(r) k_2(2k_F r) r^2 dr$$

The exchange integral containing  $V_3(r)$  has already been obtained while deriving that for  $V_2(r)$

viz

$$\frac{2k_F^5}{\pi} \int_0^\infty V_3(r) k_3(2k_F r) r^2 dr \quad (30)$$

## APPENDIX 2A

Legendre expansion for Gaussian terms in Volkov potential

We require from the expansion

$$e^{-\alpha|\mathbf{r}-\mathbf{r}'|^2} = \sum_{n=0}^{\infty} v_{\lambda}(\mathbf{r}, \mathbf{r}') P_{\lambda}(\cos\theta), \text{ where } \cos\theta = \frac{\vec{\mathbf{r}} \cdot \vec{\mathbf{r}'}}{|\vec{\mathbf{r}}| |\vec{\mathbf{r}'}} \equiv z,$$

the expression for  $v_{\lambda}(\mathbf{r}, \mathbf{r}')$

$$v_{\lambda}(\mathbf{r}, \mathbf{r}') = \frac{2\lambda+1}{2} e^{-\alpha r^2} e^{-\alpha r'^2} \int_{-1}^{+1} e^{az} P_{\lambda}(z) dz$$

where  $a \equiv 2\alpha r r'$ . Expanding the Legendre polynomial gives

$$\int_{-1}^{+1} e^{az} P_{\lambda}(z) dz = \frac{1}{2\lambda} \sum_{\nu=0}^{\lfloor \frac{\lambda}{2} \rfloor} (-1)^{\nu} \binom{\lambda}{\nu} \binom{2\lambda-2\nu}{\lambda} \int_{-1}^{+1} e^{az} z^{\lambda-2} dz$$

Using the indefinite integral

$$e^{az} z^{\lambda-2\nu} dz = e^{az} \left[ \frac{z^{\lambda-2\nu}}{a} + \sum_{\mu=1}^{\lambda-2\nu} (-1)^{\mu} \frac{(\lambda-2\nu)!}{(\lambda-2\nu-\mu)!} \frac{z^{\lambda-2\nu-\mu}}{a^{\mu+1}} \right]$$

we get

$$v_{\lambda}(\mathbf{r}, \mathbf{r}') = \frac{2\lambda+1}{2^{\lambda+1}} \sum_{\nu=0}^{\lfloor \frac{\lambda}{2} \rfloor} (-1)^{\nu} \binom{\lambda}{\nu} \binom{2\lambda-2\nu}{\lambda} \sum_{\mu=1}^{\lambda-2\nu} \frac{(\lambda-2\nu)!}{(\lambda-2\nu-\mu)!} \frac{1}{(2\alpha)^{\mu+1}} \frac{e^{-\alpha r^2}}{r^{\mu+1}} \\ \times \left\{ (-1)^{\mu} \frac{e^{-\alpha r'^2 + 2\alpha r r'}}{r'^{\mu+1}} - (-1)^{\lambda-2} \frac{e^{-\alpha r'^2 - 2\alpha r r'}}{r'^{\mu+1}} \right\}$$



APPENDIX 2B

Subtraction of the kinetic energy of the centre of mass in finite difference form

$$\frac{\left(\sum_i \vec{p}_i\right)^2}{2Am} = -\frac{\hbar^2}{2Am} \left[ \sum_i \nabla_i^2 + 2 \sum_{i < j} \vec{\nabla}_i \cdot \vec{\nabla}_j \right]$$

The first term introduces a factor  $\left(\frac{A-1}{A}\right)$  in the single-particle kinetic energy term. For the second we use

$$\begin{aligned} \vec{\nabla} &= \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \\ &= (\hat{i} \sin \theta \cos \phi + \hat{j} \sin \theta \sin \phi + \hat{k} \cos \theta) \frac{\partial}{\partial r} + (\hat{i} \cos \theta \cos \phi + \hat{j} \cos \theta \sin \phi - \hat{k} \sin \theta) \frac{1}{r} \frac{\partial}{\partial \theta} \\ &+ (-\hat{i} \sin \phi + \hat{j} \cos \phi) \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \end{aligned}$$

Define the energy unit  $E_0 = \frac{\hbar^2}{m}$ . Then

$$\frac{-\hbar^2}{2Am} \sum_{ij}^{\neq} \vec{\nabla}_i \cdot \vec{\nabla}_j = -\frac{E_0}{2A} \sum_{ij}^{\neq} \vec{\nabla}_i \cdot \vec{\nabla}_j \quad \text{gives two-particle terms involving the}$$

operator

$$\begin{aligned} \vec{\nabla}_1 \cdot \vec{\nabla}_2 &= \left[ \sin \theta_1 \cos \phi_1 \frac{\partial}{\partial r_1} + \cos \theta_1 \cos \phi_1 \frac{1}{r_1} \frac{\partial}{\partial \theta_1} - \sin \phi_1 \frac{1}{r_1 \sin \theta_1} \frac{\partial}{\partial \phi_1} \right] \\ &\left[ \sin \theta_2 \cos \phi_2 \frac{\partial}{\partial r_2} + \cos \theta_2 \cos \phi_2 \frac{1}{r_2} \frac{\partial}{\partial \theta_2} - \sin \phi_2 \frac{1}{r_2 \sin \theta_2} \frac{\partial}{\partial \phi_2} \right] \\ &+ \left[ \sin \theta_1 \sin \phi_1 \frac{\partial}{\partial r_1} + \cos \theta_1 \sin \phi_1 \frac{1}{r_1} \frac{\partial}{\partial \theta_1} + \cos \phi_1 \frac{1}{r_1 \sin \theta_1} \frac{\partial}{\partial \phi_1} \right] \\ &\left[ \sin \theta_2 \sin \phi_2 \frac{\partial}{\partial r_2} + \cos \theta_2 \sin \phi_2 \frac{1}{r_2} \frac{\partial}{\partial \theta_2} + \cos \phi_2 \frac{1}{r_2 \sin \theta_2} \frac{\partial}{\partial \phi_2} \right] \\ &+ \left[ \cos \theta_1 \frac{\partial}{\partial r_1} - \sin \theta_1 \frac{1}{r_1} \frac{\partial}{\partial \theta_1} \right] \cdot \left[ \cos \theta_2 \frac{\partial}{\partial r_2} - \sin \theta_2 \frac{1}{r_2} \frac{\partial}{\partial \theta_2} \right] \end{aligned}$$

This gives additional terms in the radial HF equations, multiplied by  $\frac{E_0}{A}$ ,

$$\begin{aligned}
& \int P_\beta(r') \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \left( \sin\theta' \cos\phi' \frac{\partial}{\partial r'} + \cos\theta' \cos\phi' \frac{1}{r'} \frac{\partial}{\partial\theta'} - \sin\phi' \frac{1}{r' \sin\theta'} \frac{\partial}{\partial\phi'} \right) \\
& Y_{\ell\beta}^{m\beta}(\theta', \phi') \sin\theta' d\theta' d\phi' P_\beta(r') dr' \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \left( \sin\theta \cos\phi \frac{\partial}{\partial r} + \cos\theta \cos\phi \frac{1}{r} \frac{\partial}{\partial\theta} \right. \\
& \left. - \sin\phi \frac{1}{r \sin\theta} \frac{\partial}{\partial\phi} \right) Y_{\ell\alpha}^{m\alpha}(\theta, \phi) \sin\theta d\theta d\phi P_\alpha(r) + \int P_\beta(r') \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \left( \sin\theta' \sin\phi' \frac{\partial}{\partial r'} \right. \\
& \left. + \cos\theta' \sin\phi' \frac{1}{r'} \frac{\partial}{\partial\theta'} + \cos\phi' \frac{1}{r' \sin\theta'} \frac{\partial}{\partial\phi'} \right) Y_{\ell\beta}^{m\beta}(\theta', \phi') \sin\theta' d\theta' d\phi' P_\beta(r') dr'. \\
& \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \left( \sin\theta \sin\phi \frac{\partial}{\partial r} + \cos\theta \sin\phi \frac{1}{r} \frac{\partial}{\partial\theta} + \cos\phi \frac{1}{r \sin\theta} \frac{\partial}{\partial\phi} \right) Y_{\ell\alpha}^{m\alpha}(\theta, \phi) \sin\theta d\theta d\phi P_\alpha(r) \\
& + \int P_\beta(r') \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \left( \cos\theta' \frac{\partial}{\partial r'} - \sin\theta' \frac{1}{r'} \frac{\partial}{\partial\theta'} \right) Y_{\ell\beta}^{m\beta}(\theta', \phi') \sin\theta' d\theta' d\phi' P_\beta(r') dr'. \\
& \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \left( \cos\theta \frac{\partial}{\partial r} - \sin\theta \frac{1}{r} \frac{\partial}{\partial\theta} \right) Y_{\ell\alpha}^{m\alpha}(\theta, \phi) \sin\theta d\theta d\phi P_\alpha(r) - \\
& \left[ \int P_\beta(r') \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \left( \sin\theta' \cos\phi' \frac{\partial}{\partial r'} + \cos\theta' \cos\phi' \frac{1}{r'} \frac{\partial}{\partial\theta'} - \sin\phi' \frac{1}{r' \sin\theta'} \frac{\partial}{\partial\phi'} \right) \right. \\
& Y_{\ell\alpha}^{m\alpha}(\theta', \phi') \sin\theta' d\theta' d\phi' P_\alpha(r') dr' \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \left( \sin\theta \cos\phi \frac{\partial}{\partial r} + \cos\theta \cos\phi \frac{1}{r} \frac{\partial}{\partial\theta} \right. \\
& \left. - \sin\phi \frac{1}{r \sin\theta} \frac{\partial}{\partial\phi} \right) Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi P_\beta(r) + \int P_\beta(r') \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \\
& \left( \sin\theta' \sin\phi' \frac{\partial}{\partial r'} + \cos\theta' \sin\phi' \frac{1}{r'} \frac{\partial}{\partial\theta'} + \cos\phi' \frac{1}{r' \sin\theta'} \frac{\partial}{\partial\phi'} \right) Y_{\ell\alpha}^{m\alpha}(\theta', \phi') \sin\theta' d\theta' d\phi' \\
& P_\alpha(r') dr' \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \left( \sin\theta \sin\phi \frac{\partial}{\partial r} + \cos\theta \sin\phi \frac{1}{r} \frac{\partial}{\partial\theta} + \cos\phi \frac{1}{r \sin\theta} \frac{\partial}{\partial\phi} \right) Y_{\ell\beta}^{m\beta}(\theta, \phi) \\
& \sin\theta d\theta d\phi P_\beta(r) + \int P_\beta(r') \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \left( \cos\theta' \frac{\partial}{\partial r'} - \sin\theta' \frac{1}{r'} \frac{\partial}{\partial\theta'} \right) Y_{\ell\alpha}^{m\alpha}(\theta', \phi') \\
& \sin\theta d\theta d\phi P_\alpha(r') dr' \int Y_{\ell\beta}^{m\beta*}(\theta, \phi) \left( \cos\theta \frac{\partial}{\partial r} - \sin\theta \frac{1}{r} \frac{\partial}{\partial\theta} \right) Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi P_\beta(r) \left. \right] \delta_{\alpha\beta}^{\sigma\tau}
\end{aligned}$$

Define the radial integrals

$$R_{\beta\alpha} \equiv \int P_\beta(r) \frac{1}{r} P_\alpha(r) dr$$

$$S_{\beta\alpha} \equiv \int P_\beta(r) \frac{\partial}{\partial r} P_\alpha(r) dr$$

Using  $r = \frac{p}{1-cp}$  and  $\frac{\partial}{\partial r} = (1-cp)^2 \frac{\partial}{\partial p}$

$$R_{\beta\alpha} = \int P_{\beta}(p) \frac{(1-cp)}{p(1-cp)^4} P_{\alpha}(p) dp = h \sum_{j=1}^{m-1} \frac{P_{\beta}^j P_{\alpha}^j}{jh(1-cjh)^3}$$

$$R_{\beta\alpha} = \sum_{j=1}^{m-1} \frac{P_{\beta}^j P_{\alpha}^j}{j(1-cjh)^3}$$

In finite difference form  $\left(\frac{\partial P_{\alpha}}{\partial p}\right)_{p=jh} = \frac{1}{2h} (P_{\alpha}^{j+1} - P_{\alpha}^{j-1})$

$$S_{\beta\alpha} = h \sum_{j=1}^{m-1} \frac{P_{\beta}^j}{(1-cjh)^4} \frac{1}{2h} (P_{\alpha}^{j+1} - P_{\alpha}^{j-1}) (1-cjh)^2$$

$$S_{\beta\alpha} = \frac{1}{2} \sum_{j=1}^{m-1} \frac{P_{\beta}^j P_{\alpha}^{j+1} - P_{\beta}^j P_{\alpha}^{j-1}}{(1-cjh)^2}$$

$$\begin{aligned} & \left[ \int Y_{\ell_{\beta}}^{m_{\beta}^*}(\theta', \phi') \sin\theta' \cos\phi' Y_{\ell_{\beta}}^m(\theta', \phi') \sin\theta' d\theta' d\phi' S_{\beta\beta} + \int Y_{\ell_{\beta}}^{m_{\beta}^*}(\theta', \phi') \cos\theta' \cos\phi' \right. \\ & \left. \frac{\partial}{\partial\theta'} Y_{\ell_{\beta}}^m(\theta', \phi') \sin\theta' d\theta' d\phi' R_{\beta\beta} - \int Y_{\ell_{\beta}}^{m_{\beta}^*}(\theta', \phi') \frac{\sin\phi'}{\sin\theta'} \frac{\partial}{\partial\phi'} Y_{\ell_{\beta}}^m(\theta', \phi') \sin\theta' d\theta' d\phi' R_{\beta\beta} \right] \times \\ & \left[ \int Y_{\ell_{\alpha}}^{m_{\alpha}^*}(\theta, \phi) \sin\theta \cos\phi Y_{\ell_{\alpha}}^{m_{\alpha}}(\theta, \phi) \sin\theta d\theta d\phi \frac{\partial P_{\alpha}}{\partial r} + \int Y_{\ell_{\alpha}}^{m_{\alpha}^*}(\theta, \phi) \cos\theta \cos\phi \frac{\partial}{\partial\theta} Y_{\ell_{\alpha}}^{m_{\alpha}}(\theta, \phi) \right. \\ & \left. \sin\theta d\theta d\phi \frac{P_{\alpha}}{r} - \int Y_{\ell_{\alpha}}^{m_{\alpha}^*}(\theta, \phi) \frac{\sin\phi}{\sin\theta} \frac{\partial}{\partial\phi} Y_{\ell_{\alpha}}^{m_{\alpha}}(\theta, \phi) \sin\theta d\theta d\phi \frac{P_{\alpha}}{r} \right] \\ & + \left[ \int Y_{\ell_{\beta}}^{m_{\beta}^*}(\theta', \phi') \sin\theta' \sin\phi' Y_{\ell_{\beta}}^m(\theta', \phi') \sin\theta' d\theta' d\phi' S_{\beta\beta} + \int Y_{\ell_{\beta}}^{m_{\beta}^*}(\theta', \phi') \cos\theta' \sin\phi' \right. \\ & \left. \frac{\partial}{\partial\theta'} Y_{\ell_{\beta}}^m(\theta', \phi') \sin\theta' d\theta' d\phi' R_{\beta\beta} + \int Y_{\ell_{\beta}}^{m_{\beta}^*}(\theta', \phi') \frac{\cos\phi'}{\sin\theta'} \frac{\partial}{\partial\phi'} Y_{\ell_{\beta}}^m(\theta', \phi') \sin\theta' d\theta' d\phi' R_{\beta\beta} \right] \times \\ & \left[ \int Y_{\ell_{\alpha}}^{m_{\alpha}^*}(\theta, \phi) \sin\theta \sin\phi Y_{\ell_{\alpha}}^{m_{\alpha}}(\theta, \phi) \sin\theta d\theta d\phi \frac{\partial P_{\alpha}}{\partial r} + \int Y_{\ell_{\alpha}}^{m_{\alpha}^*}(\theta, \phi) \cos\theta \sin\phi \frac{\partial}{\partial\theta} Y_{\ell_{\alpha}}^m(\theta, \phi) \right. \\ & \left. \sin\theta d\theta d\phi \frac{P_{\alpha}}{r} + \int Y_{\ell_{\alpha}}^{m_{\alpha}^*}(\theta, \phi) \frac{\cos\phi}{\sin\theta} \frac{\partial}{\partial\phi} Y_{\ell_{\alpha}}^{m_{\alpha}}(\theta, \phi) \sin\theta d\theta d\phi \frac{P_{\alpha}}{r} \right] \\ & + \left[ \int Y_{\ell_{\beta}}^{m_{\beta}^*}(\theta', \phi') \cos\theta' Y_{\ell_{\beta}}^m(\theta', \phi') \sin\theta' d\theta' d\phi' S_{\beta\beta} - \int Y_{\ell_{\beta}}^{m_{\beta}^*}(\theta', \phi') \sin\theta' \frac{\partial}{\partial\theta'} Y_{\ell_{\beta}}^m(\theta', \phi') \right. \\ & \left. R_{\beta\beta} \right] \\ & \times \left[ \int Y_{\ell_{\alpha}}^{m_{\alpha}^*}(\theta, \phi) \cos\theta Y_{\ell_{\alpha}}^{m_{\alpha}}(\theta, \phi) \sin\theta d\theta d\phi \frac{\partial P_{\alpha}}{\partial r} - \int Y_{\ell_{\alpha}}^{m_{\alpha}^*}(\theta, \phi) \sin\theta \frac{\partial}{\partial\theta} Y_{\ell_{\alpha}}^{m_{\alpha}}(\theta, \phi) \sin\theta d\theta d\phi \frac{P_{\alpha}}{r} \right] \end{aligned}$$

$$\begin{aligned}
& - \delta_{\alpha\beta}^{\sigma\tau} \left[ \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \sin\theta' \cos\phi' Y_{\ell\beta}^{m\beta}(\theta', \phi') \sin\theta' d\theta' d\phi' S_{\beta\alpha} + \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \cos\theta' \cos\phi' \right. \\
& \left. \frac{\partial}{\partial\theta'} Y_{\ell\alpha}^{m\alpha}(\theta', \phi') \sin\theta' d\theta' d\phi' R_{\beta\alpha} - \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \frac{\sin\phi'}{\sin\theta'} \frac{\partial}{\partial\phi'} Y_{\ell\alpha}^{m\alpha}(\theta', \phi') \sin\theta' d\theta' d\phi' R_{\beta\alpha} \right] \\
& \times \left[ \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \sin\theta \cos\phi Y_{\ell\alpha}^{m\alpha}(\theta, \phi) \sin\theta d\theta d\phi \frac{\partial P_{\beta}}{\partial r} + \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \cos\theta \cos\phi \frac{\partial}{\partial\theta} Y_{\ell\alpha}^{m\alpha}(\theta, \phi) \right. \\
& \left. \sin\theta d\theta d\phi \frac{P_{\beta}}{r} - \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \frac{\sin\phi}{\sin\theta} \frac{\partial}{\partial\phi} Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi \frac{P_{\beta}}{r} \right] \\
& - \delta_{\alpha\beta}^{\sigma\tau} \left[ \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \sin\theta' \sin\phi' Y_{\ell\beta}^{m\beta}(\theta', \phi') \sin\theta' d\theta' d\phi' S_{\beta\alpha} + \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \cos\theta' \sin\phi' \right. \\
& \left. \frac{\partial}{\partial\theta'} Y_{\ell\alpha}^{m\alpha}(\theta', \phi') \sin\theta' d\theta' d\phi' R_{\beta\alpha} + \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \frac{\cos\phi'}{\sin\theta'} \frac{\partial}{\partial\phi'} Y_{\ell\alpha}^{m\alpha}(\theta', \phi') \sin\theta' d\theta' d\phi' R_{\beta\alpha} \right] \times \\
& \times \left[ \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \sin\theta \sin\phi Y_{\ell\alpha}^{m\alpha}(\theta, \phi) \sin\theta d\theta d\phi \frac{\partial P_{\beta}}{\partial r} + \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \cos\theta \sin\phi \frac{\partial}{\partial\theta} Y_{\ell\beta}^{m\beta}(\theta, \phi) \right. \\
& \left. \sin\theta d\theta d\phi \frac{P_{\beta}}{r} + \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \frac{\cos\phi}{\sin\theta} \frac{\partial}{\partial\phi} Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi \frac{P_{\beta}}{r} \right] \\
& - \delta_{\alpha\beta}^{\sigma\tau} \left[ \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \cos\theta' Y_{\ell\alpha}^{m\alpha}(\theta', \phi') \sin\theta' d\theta' d\phi' S_{\beta\alpha} - \int Y_{\ell\beta}^{m\beta*}(\theta', \phi') \sin\theta' \frac{\partial}{\partial\theta'} \right. \\
& \left. Y_{\ell\alpha}^{m\alpha}(\theta', \phi') \sin\theta' d\theta' d\phi' R_{\beta\alpha} \right] \times \left[ \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \cos\theta Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi \frac{\partial P_{\beta}}{\partial r} \right. \\
& \left. - \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \sin\theta \frac{\partial}{\partial\theta} Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi \frac{P_{\beta}}{r} \right]
\end{aligned}$$

Define the angular integrals  $A_{\alpha\beta}^{(n)}$

$$\begin{aligned}
A_{\alpha\beta}^{(1)} &= \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \sin\theta \cos\phi Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi \\
A_{\alpha\beta}^{(2)} &= \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \cos\theta \cos\phi \frac{\partial}{\partial\theta} Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi \\
A_{\alpha\beta}^{(3)} &= \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \frac{\sin\phi}{\sin\theta} \frac{\partial}{\partial\phi} Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi \\
A_{\alpha\beta}^{(4)} &= i \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \sin\theta \sin\phi Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi \\
A_{\alpha\beta}^{(5)} &= i \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \cos\theta \sin\phi \frac{\partial}{\partial\theta} Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi \\
A_{\alpha\beta}^{(6)} &= i \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \frac{\cos\phi}{\sin\theta} \frac{\partial}{\partial\phi} Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi
\end{aligned}$$

$$A_{\alpha\beta}^{(7)} = \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \cos\theta Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi$$

$$A_{\alpha\beta}^{(8)} = \int Y_{\ell\alpha}^{m\alpha*}(\theta, \phi) \sin\theta \frac{\partial}{\partial\theta} Y_{\ell\beta}^{m\beta}(\theta, \phi) \sin\theta d\theta d\phi$$

$$\begin{aligned} & \left[ A_{\beta\beta}^{(1)} S_{\beta\beta} + A_{\beta\beta}^{(2)} R_{\beta\beta} - A_{\beta\beta}^{(3)} R_{\beta\beta} \right] \times \left[ A_{\alpha\alpha}^{(1)} \frac{\partial P_\alpha}{\partial r} + A_{\alpha\alpha}^{(2)} \frac{P_\alpha}{r} - A_{\alpha\alpha}^{(3)} \frac{P_\alpha}{r} \right] \\ & - \left[ A_{\beta\beta}^{(4)} S_{\beta\beta} + A_{\beta\beta}^{(5)} R_{\beta\beta} + A_{\beta\beta}^{(6)} R_{\beta\beta} \right] \times \left[ A_{\alpha\alpha}^{(4)} \frac{\partial P_\alpha}{\partial r} + A_{\alpha\alpha}^{(5)} \frac{P_\alpha}{r} + A_{\alpha\alpha}^{(6)} \frac{P_\alpha}{r} \right] \\ & + \left[ A_{\beta\beta}^{(7)} S_{\beta\beta} - A_{\beta\beta}^{(8)} R_{\beta\beta} \right] \times \left[ A_{\alpha\alpha}^{(7)} \frac{\partial P_\alpha}{\partial r} - A_{\alpha\alpha}^{(8)} \frac{P_\alpha}{r} \right] \\ & - \delta_{\alpha\beta} \sigma_T \left[ A_{\beta\alpha}^{(1)} S_{\beta\alpha} + A_{\beta\alpha}^{(2)} R_{\beta\alpha} - A_{\beta\alpha}^{(3)} R_{\beta\alpha} \right] \times \left[ A_{\alpha\beta}^{(1)} \frac{\partial P_\beta}{\partial r} + A_{\alpha\beta}^{(2)} \frac{P_\beta}{r} - A_{\alpha\beta}^{(3)} \frac{P_\beta}{r} \right] \\ & + \delta_{\alpha\beta} \sigma_T \left[ A_{\beta\alpha}^{(4)} S_{\beta\alpha} + A_{\beta\alpha}^{(5)} R_{\beta\alpha} + A_{\beta\alpha}^{(6)} R_{\beta\alpha} \right] \times \left[ A_{\alpha\beta}^{(4)} \frac{\partial P_\beta}{\partial r} + A_{\alpha\beta}^{(5)} \frac{P_\beta}{r} + A_{\alpha\beta}^{(6)} \frac{P_\beta}{r} \right] \\ & - \delta_{\alpha\beta} \sigma_T \left[ A_{\beta\alpha}^{(7)} S_{\beta\alpha} - A_{\beta\alpha}^{(8)} R_{\beta\alpha} \right] \times \left[ A_{\alpha\beta}^{(7)} \frac{\partial P_\beta}{\partial r} - A_{\alpha\beta}^{(8)} \frac{P_\beta}{r} \right] \\ & = \left[ A_{\alpha\alpha}^{(1)} (A_{\beta\beta}^{(1)} S_{\beta\beta} + A_{\beta\beta}^{(2)} R_{\beta\beta} - A_{\beta\beta}^{(3)} R_{\beta\beta}) - A_{\alpha\alpha}^{(4)} (A_{\beta\beta}^{(4)} S_{\beta\beta} + A_{\beta\beta}^{(5)} R_{\beta\beta} + A_{\beta\beta}^{(6)} R_{\beta\beta}) + A_{\alpha\alpha}^{(7)} (A_{\beta\beta}^{(7)} S_{\beta\beta} \right. \\ & \left. - A_{\beta\beta}^{(8)} R_{\beta\beta}) \right] \frac{\partial P_\alpha}{\partial r} \\ & + \left[ (A_{\alpha\alpha}^{(2)} - A_{\alpha\alpha}^{(3)}) (A_{\beta\beta}^{(1)} S_{\beta\beta} + A_{\beta\beta}^{(2)} R_{\beta\beta} - A_{\beta\beta}^{(3)} R_{\beta\beta}) + (A_{\alpha\alpha}^{(5)} + A_{\alpha\alpha}^{(6)}) (A_{\beta\beta}^{(4)} S_{\beta\beta} + A_{\beta\beta}^{(5)} R_{\beta\beta} + A_{\beta\beta}^{(6)} R_{\beta\beta}) \right. \\ & \left. - A_{\alpha\alpha}^{(8)} (A_{\beta\beta}^{(7)} S_{\beta\beta} - A_{\beta\beta}^{(8)} R_{\beta\beta}) \right] \frac{P_\alpha}{r} \\ & - \delta_{\alpha\beta} \sigma_T \left[ A_{\alpha\beta}^{(1)} (A_{\beta\alpha}^{(1)} S_{\beta\alpha} + A_{\beta\alpha}^{(2)} R_{\beta\alpha} - A_{\beta\alpha}^{(3)} R_{\beta\alpha}) - A_{\alpha\beta}^{(4)} (A_{\beta\alpha}^{(4)} S_{\beta\alpha} + A_{\beta\alpha}^{(5)} R_{\beta\alpha} + A_{\beta\alpha}^{(6)} R_{\beta\alpha}) \right. \\ & \left. + A_{\alpha\beta}^{(7)} (A_{\beta\alpha}^{(7)} S_{\beta\alpha} - A_{\beta\alpha}^{(8)} R_{\beta\alpha}) \right] \frac{\partial P_\beta}{\partial r} \\ & - \delta_{\alpha\beta} \sigma_T \left[ A_{\alpha\beta}^{(2)} - A_{\alpha\beta}^{(3)} \right] (A_{\beta\alpha}^{(1)} S_{\beta\alpha} + A_{\beta\alpha}^{(2)} R_{\beta\alpha} - A_{\beta\alpha}^{(3)} R_{\beta\alpha}) - (A_{\alpha\beta}^{(5)} + A_{\alpha\beta}^{(6)}) (A_{\beta\alpha}^{(4)} S_{\beta\alpha} + A_{\beta\alpha}^{(5)} R_{\beta\alpha} \\ & \left. + A_{\beta\alpha}^{(6)} R_{\beta\alpha}) - A_{\alpha\beta}^{(8)} (A_{\beta\alpha}^{(7)} S_{\beta\alpha} - A_{\beta\alpha}^{(8)} R_{\beta\alpha}) \right] \frac{P_\beta}{r} \\ \text{Define } K_{\alpha\beta} & \equiv A_{\alpha\alpha}^{(1)} (A_{\beta\beta}^{(1)} S_{\beta\beta} + A_{\beta\beta}^{(2)} R_{\beta\beta} - A_{\beta\beta}^{(3)} R_{\beta\beta}) - A_{\alpha\alpha}^{(4)} (A_{\beta\beta}^{(4)} S_{\beta\beta} + A_{\beta\beta}^{(5)} R_{\beta\beta} + A_{\beta\beta}^{(6)} R_{\beta\beta}) \end{aligned}$$

$$+ A_{\alpha\alpha}^{(7)} (A_{\beta\beta}^{(7)} S_{\beta\beta} - A_{\beta\beta}^{(8)} R_{\beta\beta})$$

$$L_{\alpha\beta} \equiv (A_{\alpha\alpha}^{(2)} - A_{\alpha\alpha}^{(3)}) (A_{\beta\beta}^{(1)} S_{\beta\beta} + A_{\beta\beta}^{(2)} R_{\beta\beta} - A_{\beta\beta}^{(3)} R_{\beta\beta}) - (A_{\alpha\alpha}^{(5)} + A_{\alpha\alpha}^{(6)}) (A_{\beta\beta}^{(4)} S_{\beta\beta} + A_{\beta\beta}^{(5)} R_{\beta\beta} + A_{\beta\beta}^{(6)} R_{\beta\beta}) - A_{\alpha\alpha}^{(8)} (A_{\beta\beta}^{(7)} S_{\beta\beta} - A_{\beta\beta}^{(8)} R_{\beta\beta})$$

$$M_{\alpha\beta} \equiv A_{\alpha\beta}^{(1)} (A_{\beta\alpha}^{(1)} S_{\beta\alpha} + A_{\beta\alpha}^{(2)} R_{\beta\alpha} - A_{\beta\alpha}^{(3)} R_{\beta\alpha}) - A_{\alpha\beta}^{(4)} (A_{\beta\alpha}^{(4)} S_{\beta\alpha} + A_{\beta\alpha}^{(5)} R_{\beta\alpha} + A_{\beta\alpha}^{(6)} R_{\beta\alpha}) + A_{\alpha\beta}^{(7)} (A_{\beta\alpha}^{(7)} S_{\beta\alpha} - A_{\beta\alpha}^{(8)} R_{\beta\alpha})$$

$$N_{\alpha\beta} \equiv (A_{\alpha\beta}^{(2)} - A_{\alpha\beta}^{(3)}) (A_{\beta\alpha}^{(1)} S_{\beta\alpha} + A_{\beta\alpha}^{(2)} R_{\beta\alpha} - A_{\beta\alpha}^{(3)} R_{\beta\alpha}) - (A_{\alpha\beta}^{(5)} + A_{\alpha\beta}^{(6)}) (A_{\beta\alpha}^{(4)} S_{\beta\alpha} + A_{\beta\alpha}^{(5)} R_{\beta\alpha} + A_{\beta\alpha}^{(6)} R_{\beta\alpha}) - A_{\alpha\beta}^{(8)} (A_{\beta\alpha}^{(7)} S_{\beta\alpha} - A_{\beta\alpha}^{(8)} R_{\beta\alpha})$$

$$\text{giving } \left( K_{\alpha\beta} \frac{\partial P}{\partial r} + L_{\alpha\beta} \frac{P}{r} \right) - \delta_{\alpha\beta}^{\sigma\tau} \left( M_{\alpha\beta} \frac{\partial P}{\partial r} + N_{\alpha\beta} \frac{P}{r} \right)$$

At mesh point  $k$  this gives

$$K_{\alpha\beta} (1-ckh)^2 \frac{1}{2h} (P_{\alpha}^{k+1} - P_{\alpha}^{k-1}) + L_{\alpha\beta} \left( \frac{1-ckh}{kh} \right) P_{\alpha}^k - \delta_{\alpha\beta}^{\sigma\tau} \left( M_{\alpha\beta} \frac{(1-ckh)^2}{2h} (P_{\beta}^{k+1} - P_{\beta}^{k-1}) + N_{\alpha\beta} \left( \frac{1-ckh}{kh} \right) P_{\beta}^k \right)$$

Define

$$K_{\alpha} \equiv \sum_{\beta} K_{\alpha\beta}$$

$$L_{\alpha} \equiv \sum_{\beta} L_{\alpha\beta}$$

$$M_{\alpha}^k \equiv \sum_{\beta} \delta_{\alpha\beta}^{\sigma\tau} M_{\alpha\beta} (P_{\beta}^{k+1} - P_{\beta}^{k-1})$$

$$N_{\alpha}^k \equiv \sum_{\beta} \delta_{\alpha\beta}^{\sigma\tau} N_{\alpha\beta} P_{\beta}^k$$

The radial equations at each mesh point with centre of mass correction are

$$- \frac{E_0}{2h^2} (P_{\alpha}^{k-1} + P_{\alpha}^{k+1}) + \left| \frac{E_0}{h^2} + \frac{E_0 \ell_{\alpha} (\ell_{\alpha} + 1)}{2k^2 h^2 (1-ckh)^2} + \frac{y_{\alpha}^k}{(1-ckh)^4} - \frac{P_{\alpha}^k}{(1-ckh)^4} \right| P_{\alpha}^k + \frac{x_{\alpha}^k}{(1-ckh)^4}$$

$$\begin{aligned}
& + \frac{E_0}{2h^2} \frac{1}{A} (P_\alpha^{k-1} + P_\alpha^{k+1}) - \frac{1}{A} \left[ \frac{E_0}{h^2} + \frac{E_0 \ell_\alpha (\ell_\alpha + 1)}{2k^2 h^2 (1-ckh)^2} \right] P_\alpha^k + \frac{E_0}{A} K_\alpha \frac{1}{2h(1-ckh)^2} (P_\alpha^{k+1} - P_\alpha^{k-1}) \\
& + \frac{E_0}{A} L_\alpha \frac{1}{kh(1-ckh)^3} P_\alpha^k - \frac{E_0}{A} M_\alpha^k \frac{1}{2h(1-ckh)^2} - \frac{E_0}{A} N_\alpha^k \frac{1}{kh(1-ckh)^3} = 0 \\
& = \left( \frac{-E_0}{2h^2} + \frac{E_0}{2h^2 A} - \frac{E_0 K_\alpha}{2h(1-ckh)^2 A} \right) P_\alpha^{k-1} + \left( \frac{-E_0}{2h^2} + \frac{E_0}{2h^2 A} + \frac{E_0 K_\alpha}{2h^2(1-ckh)^2 A} \right) P_\alpha^{k+1} \\
& + \left( \frac{E_0}{h^2} - \frac{E_0}{h^2 A} + \frac{E_0 \ell_\alpha (\ell_\alpha + 1)}{2k^2 h^2 (1-ckh)^2} - \frac{E_0 \ell_\alpha (\ell_\alpha + 1)}{2k^2 h^2 (1-ckh)^2 A} + \frac{Y_\alpha^k}{(1-ckh)^4} + \frac{E_0 L_\alpha}{kh(1-ckh)^3 A} \right. \\
& \left. - \frac{P_\alpha^M}{(1-ckh)^4} \right) P_\alpha^k + \frac{X_\alpha^k}{(1-ckh)^4} - \frac{E_0 M_\alpha^k}{2h(1-ckh)^2 A} - \frac{E_0 N_\alpha^k}{kh(1-ckh)^3 A} = 0 \\
f_\alpha^k & = \left[ \frac{-E_0}{2h^2} \left( \frac{A-1}{A} \right) - \frac{E_0 K_\alpha}{2h(1-ckh)^2 A} \right] P_\alpha^{k-1} + \left[ \frac{-E_0}{2h^2} \left( \frac{A-1}{A} \right) + \frac{E_0 K_\alpha}{2h(1-ckh)^2 A} \right] P_\alpha^{k+1} \\
& + \left[ \left( \frac{E_0}{h^2} + \frac{E_0 \ell_\alpha (\ell_\alpha + 1)}{2k^2 h^2 (1-ckh)^2} \right) \left( \frac{A-1}{A} \right) + \frac{E_0 L_\alpha}{kh(1-ckh)^3 A} + \frac{Y_\alpha^k}{(1-ckh)^4} - \frac{P_\alpha^M}{(1-ckh)^4} \right] P_\alpha^k \\
& + \left[ \frac{X_\alpha^k}{(1-ckh)^4} - \frac{E_0 M_\alpha^k}{2h(1-ckh)^2 A} - \frac{E_0 N_\alpha^k}{kh(1-ckh)^3 A} \right] = 0 \quad 1 \leq k \leq M-1 \\
& = J_{k,k-1} P_\alpha^{k-1} + J_{k,k+1} P_\alpha^{k+1} + J_{kk} P_\alpha^k + \left[ \frac{X_\alpha^k}{(1-ckh)^4} - \frac{E_0}{A} \left( \frac{M_\alpha^k}{2h(1-ckh)^2} + \frac{N_\alpha^k}{kh(1-ckh)^3} \right) \right] = 0 \\
J_{k,k-1} & = - \frac{E_0}{2h^2} \left( \frac{A-1}{A} \right) - \frac{E_0 K_\alpha}{2h(1-ckh)^2 A} \\
J_{k,k+1} & = - \frac{E_0}{2h^2} \left( \frac{A-1}{A} \right) + \frac{E_0 K_\alpha}{2h(1-ckh)^2 A} \\
J_{kk} & = \left( \frac{E_0}{h^2} + \frac{E_0 \ell_\alpha (\ell_\alpha + 1)}{2k^2 h^2 (1-ckh)^2} \right) \left( \frac{A-1}{A} \right) + \frac{E_0 L_\alpha}{kh(1-ckh)^3 A} + \frac{Y_\alpha^k}{(1-ckh)^4} - \frac{P_\alpha^M}{(1-ckh)^4}
\end{aligned}$$





except for the last (i.e.  $k=m$ ) one which is

$$\left( \frac{2}{h^2} + \frac{P_{2M+1} P_{2M+2} e^{-kh/P_{2M+2}}}{kh} - \frac{e^{-\alpha h}}{h^2} \right) e^{-\alpha R} \left( \frac{\sqrt{8} P_{2M+3} P_{2M+4} e^{-kh/P_{2M+4}}}{kh} \right) e^{-\alpha R}$$

$$\left( \frac{\sqrt{8} P_{2M+3} P_{2M+4} e^{-kh/P_{2M+4}}}{kh} \right) e^{-\alpha R} \left( \frac{2}{h^2} + \frac{6}{k^2 h^2} + \frac{P_{2M+1} P_{2M+2} e^{-kh/P_{2M+2}}}{kh} \right.$$

$$\left. - \frac{2P_{2M+3} P_{2M+4} e^{-kh/P_{2M+4}}}{kh} - \frac{e^{-\alpha h}}{h^2} \right) e^{-\alpha R}$$

The matrix B is  $(2M \times 4)$ -dimensional and the four columns of B are given as follows :

1st column

$$\frac{P_{2M+2} e^{-kh/P_{2M+2}} P_{\ell k}}{kh} \quad \text{for } \ell=1,2 \text{ and } k=1,2,\dots,M-1$$

and when  $k=M$ , the above is multiplied by  $e^{-\alpha R}$ .

2nd column

$$\frac{P_{2M+1} e^{-kh/P_{2M+2}}}{kh} + \frac{P_{2M+1} e^{-kh/P_{2M+2}}}{P_{2M+2}} \quad \text{for } \ell=1,2 \text{ and } k=1,2,\dots,M-1$$

and again this is multiplied by  $e^{-\alpha R}$  for  $k=M$ .

3rd column

$$\frac{\sqrt{8} P_{2M+4} e^{-kh/P_{2M+4}}}{kh} P_{\ell+1,k} \quad \text{for } \ell=1 \text{ and } k=1,2,\dots,M-1, \text{ and multiplied}$$

by  $e^{-\alpha R}$  when  $k=M$ .

$$-2P_{2M+4} \frac{e^{-kh/P_{2M+4}}}{kh} P_{\ell k} + \sqrt{8} P_{2M+4} \frac{e^{-kh/P_{2M+4}}}{kh} P_{\ell-1,k} \quad \text{for } \ell=2 \text{ and } k=1,2,\dots,M-1,$$

and multiplied by  $e^{-\alpha R}$  for  $k=M$ .

4th column

$$\sqrt{8} \left( \frac{P_{2M+3} e^{-kh/P_{2M+4}}}{kh} + \frac{P_{2M+3}}{P_{2M+4}} e^{-kh/P_{2M+4}} \right) P_{\ell+1,k} \quad \text{for } \ell=1 \text{ and } k=1,2,\dots,M-1$$

and

$$\left( \frac{P_{2M+3} e^{-kh/P_{2M+4}}}{P_{2M+4}} + \frac{P_{2M+3}}{P_{2M+4}} e^{-kh/P_{2M+4}} \right) \left( -2P_{\ell k} + \sqrt{8} P_{\ell-1,k} \right) \quad \text{for } \ell=2 \text{ and } k=1,2,\dots,M-1.$$

For both these expressions, we multiply by  $e^{-\alpha R}$  when  $k=M$ .

The rows of the  $(4 \times 2M)$  matrix  $C$  are :

1st row

All the first row elements are zero except for the last two which are  $2P_{2M-1}$  and  $2P_{2M}$ .

2nd row

$$2P_{\ell k} \quad \ell=1,2 \text{ and } k=1,2,\dots,M-1.$$

When  $k=M$ , the elements are  $e^{-2\alpha R} \left( 1 + \frac{1}{\alpha h} \right) P_{\ell M} \quad \ell=1,2$

3rd row

$$-2P_D P_{\ell k} \quad \text{for } \ell=1 \text{ and } k=1,2,\dots,M-1$$

$$2(1-P_D) P_{\ell k} \quad \text{for } \ell=2 \text{ and } k=1,2,\dots,M-1.$$

These are multiplied by  $\frac{e^{-2\alpha R}}{2} \left( 1 + \frac{1}{\alpha h} \right)$  when  $k=M$ .

4th row

$$\frac{\sqrt{2}}{10} P_{\ell+1,k} k^2 h^2 - 2QP_{\ell k} \quad \text{if } \ell=1 \text{ and } k=1,2,\dots,M-1$$

$$\frac{\sqrt{2}}{10} P_{\ell-1,k} k^2 h^2 - 2QP_{\ell k} - \frac{1}{10} P_{\ell k} k^2 h^2 \quad \text{if } \ell=2 \text{ and } k=1,2,\dots,M-1$$

$$\frac{\sqrt{2}}{10} P_{2M} e^{-2\alpha R} \left\{ \frac{R^2}{2} \left( 1 + \frac{1}{\alpha h} \right) + \frac{R}{2\alpha^2 h} + \frac{1}{4\alpha^2 h} \right\} - Q P_{2M-1} e^{-2\alpha R} \left( 1 + \frac{1}{\alpha h} \right) \text{ for } \ell=1 \text{ and } k=M$$

$$\left( \frac{\sqrt{2}}{10} P_{2M-1} - \frac{1}{10} P_{2M} \right) e^{-2\alpha R} \left\{ \frac{R^2}{2} \left( 1 + \frac{1}{\alpha h} \right) + \frac{R}{2\alpha^2 h} + \frac{1}{4\alpha^2 h} \right\} - Q P_{2M} e^{-2\alpha R} \left( 1 + \frac{1}{\alpha h} \right) \text{ for } \ell=2 \text{ and } k=M.$$

## REFERENCES

- [1] D.R. Hartree Proc Camb Phil Soc 24 111 (1928)
  - [2] P.O. Löwdin J Math Phys 3 1171 (1962)
  - [3] P.O. Löwdin Rev Mod Phys 35 702 (1963)
  - [4] E.A. Hylleraas Z Phys 54 347 (1939)
- See also J.C. Slater "Quantum Theory of Atomic Structure" Vol 2  
McGraw-Hill (1960)
- [5] R. Jastrow Phys Rev 98 1479 (1955)
  - [6] V.J. Emery Nucl Phys 6 (1958)
  - [7] S.F. Boys, N.C. Handy Proc Roy Soc A 310 43 (1969)
  - [8] K.A. Brueckner, C.A. Levinson Phys Rev 97 1344 (1955)
  - [9] J. Goldstone Proc Roy Soc A 239 267 (1957)
  - [10] K.A. Brueckner, J.L. Gammel Phys Rev 109 1023 (1957)
  - [11] K.A. Brueckner, J.L. Gammel, H. Weitzner Phys Rev 110 431 (1958)
  - [12] J. Tharrats, O. Cerceau, O. Rojo J Math Phys 6 1315 (1964)
- F. Villars 'Proc of Int School of Phys "Enrico Fermi", Course 23  
(1961) Academic Press 1963
- [13] M.A. Preston 'Physics of the Nucleus' - Chap 9 Addison-Wesley 1962
  - [14] J.P. Elliot, A.M. Lane Encyclopedia of Physics vol 39 Springer-Verlag 1957
  - [15] L. Eisenbud, E.P. Wigner Proc Nat Acad Sci USA 27 281 (1941)
  - [16] See for example, J.M. Eisenberg, W. Greiner 'Nuclear Theory'  
vol 3 North-Holland 1972
  - [17] R. Jastrow Phys Rev 81 165 (1950)
  - [18] G.A. Baker Jr. Phys Rev 128 1485 (1962)
- S.A. Moszkowski Phys Rev 129 1901 (1963)
- A.M. Green Nucl Phys 33 218 (1962)

- [19] P. Middelstaedt Acta Phys Hung 19 303 (1965)
- [20] A.B. Volkov Nucl Phys 74 33 (1965)
- [21] H. Feshbach, J. Schwinger Phys Rev 84 194 (1951)
- [22] P. Middelstaedt, M. Ristig Z Phys 193 349 (1966)
- [23] W.H. Rohl, W. Stocker Z Phys 212 477 (1968)
- [24] M. Ristig Z Phys 199 325 (1967) - see also [22]
- [25] J.S. Bell 'Lecture Notes on the Many-Body Problem' - Bergen  
(1961) Benjamin N.Y. 1962
- [26] M. Ristig, S. Kistler Z Phys 215 419 (1968)
- [27] R.K. Bhaduri, M.A. Preston Can J Phys 42 696 (1964)
- F. Coester, S. Cohen, B. Day, C.M. Vincent Phys Rev C1 769 (1970)
- [28] M. Ristig Z Phys 232 279 (1970) - see also [24]
- [29] P.O. Löwdin J. Molec Spec 3 46 (1959)
- [30] V. Fock Z Phys 63 855 (1930)
- [31] S.J. Epstein, J.O. Hirschfelder Phys Rev 123 1495 (1961)
- [32] J.C. Slater J Chem Phys 1 687 (1933)
- [33] P.A. Seeger Nucl Phys 25 1 (1961)
- [34] J.L. Gammel, R.S. Christian, R.M. Thaler Phys Rev 105 311 (1957)
- [35] E. Merzbacher 'Quantum Mechanics' Chap 8 Wiley 1961
- [36] K. Brueckner 'The Many-Body Problem' - Les Houches (1958) Wiley 1958
- [37] E.A. Bangudu, P.D. Robinson Proc Phys Soc 86 1259 (1965)
- [38] N. Ullah, R.K. Nesbet Nucl Phys 39 239 (1962)
- [39] A de Shalit, H. Feshbach 'Theoretical Nuclear Physics' vol 1  
Chap 6 Wiley 1974
- [40] A.K. Kerman in 'Cargèse Lect in Physics' vol 3 Gordon and Breach 1969
- [41] D.M. Brink, M.E. Grypeos Nucl Phys A 97 81 (1967)
- [42] I. Talmi Helv Phys Acta 25 185 (1952)
- M. Moshinsky Nucl Phys 13 104 (1959)

- [43] I.R. Afnan, Y.C. Tang Phys Rev 175 1337 (1968)
- [44] S. Fantoni, L. Panattoni, S. Rosati Nuovo Cimento 69A 80 (1970)
- [45] S.F. Boys, N.C. Handy Proc Roy Soc A310 63 (1969)
- [46] J.K. Cayford, W.R. Fimple, D.G. Unger J Comp Phys 15 81 (1974)
- [47] L. Hulthén, M. Sugawara Encycl of Physics vol 39 Springer-Verlag  
1957
- [48] L.C. Biedenharn, J.M. Blatt, M.H. Kalos Nucl Phys 6 359 (1958)
- [49] J.S. Bell, E.J. Squires Adv in Phys 10 211 (1961)

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