LOCAL FERMI MOMENTUM DEPENDENCE IN THE EFFECTIVE NUCLEAR INTERACTION

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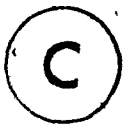

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LOCAL FERMI MOMENTUM

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ABSTRACT

We have investigated the recently proposed Local Fermi Momentum Approximation's use in the context of the Hartree-Fock model of the nucleus. This suggests the possibility that the effective nuclear potential could depend on the Local Fermi Momentum. It is shown that such a potential derives no rearrangement energy from this dependence. This fact shows why the Density Matrix Expansion Approximation treats the rearrangement energy accurately. In order to produce a rearrangement energy, the effective potential should be chosen to depend on the density as well as on the Local Fermi Momentum. This led to the development of a modified Skyrme-like force in which the density dependence is replaced by a kinetic-energy-density dependence. This force was adjusted to give good fits to observed ground-state properties of closed-shell nuclei, and of infinite nuclear matter. Its use requires that more attention be paid to the numerical solution of the Hartree-Fock problem than for a regular Skyrme force.

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CHAPTER I

INTRODUCTION

The present work will investigate some aspects of the Local Fermi Momentum (LFM) recently proposed by Campi and Bouyssy, (CB 78), as it applies to the calculation of the static properties of nuclei. In particular we have considered the LFM approximation as an alternative to the Local Density Approximation (LDA) which has been widely used previously. This prompted the development of a kinetic-energy-density dependent effective nucleon-nucleon interaction which has been successfully used in Hartree-Fock calculations of doubly-magic spherical nuclei.

In order to set a framework for this exposition, the remainder of this introduction will be devoted to a review of the relevant facts concerning: (i) the Nuclear Shell Model, (ii) Hartree-Fock calculations, (iii) the Density Matrix Expansion (DME), and (iv) Skyrme's interaction.

(i) The Nuclear Shell Model:

The shell model of the nucleus (GJ 55), (ST 63) in its simplest form provides a ready explanation for certain nuclear properties: the existence of magic numbers; properties of nuclei with one or a few active nucleons; and islands of isomerism.

It is essentially an independent-particle model, in which each nucleon is assumed to move in the self-consistent field due to all the other nucleons. The state of the nucleus is specified by the single-particle states of its constituents. these states are described by the notation $n\ell jq$, where $n \in \mathbb{N}$ is the principle quantum number; $\ell = s,p,d,f,...$ represents an orbital angular momentum quantum number of $0,1,2,3,...$; $j = \ell \pm \frac{1}{2}$ is the total angular momentum quantum number; and q is the charge index of the state.

The ordering of the single-particle levels is obtained from experiment. Of particular importance are levels separated by large energy gaps. When all levels below a gap are completely filled with neutrons (or protons), the nucleus is said to have neutron number N (or atomic number Z) "magic". Experimental evidence of the magic numbers 2, 8, 20, (28), (40), 50, 82, 126 is abundant and well known (GJ 55), (Seg 77). It is worth remarking that a spin-orbit ($\underset{\sim}{\ell}\cdot\underset{\sim}{s}$ dependent) potential is required in the single-particle Hamiltonian to explain these values beyond 20.

The self-consistent field is assumed to be spherically symmetric about the nuclear centre of mass, (which is, however, not fixed (Fri 71)).

(ii) Hartree-Fock Method:

The Hartree-Fock (HF) method (Har 28), (Foc 30) provides a framework for understanding the nuclear shell model. In par-

ticular it provides the means of calculating the self-consistent field and single-particle states.

The nuclear wavefunction is taken to be a Slater determinant:

$$\Phi(\xi_1,\cdots,\xi_A) = A^{-1/2}\det|\phi_i(\xi_j)|$$

where $A = N+Z$ is the mass number, $\{\phi_i\}$ are the single-particle states, and $\xi_j = (\underset{\sim}{r}_j,\sigma_j,q_j)$ is the coordinate of the j-th nucleon. Here $\sigma = \pm\frac{1}{2}$ is the spin projection and $q = \frac{1}{2}$ $(-\frac{1}{2})$ or p(n).

One then requires that the total energy of the nucleus $E_{TOT} = \langle\Phi|H|\Phi\rangle$ be stationary with respect to the individual variations of the ϕ_i, which are constrained to be normalized. If one assumes nucleons to interact only by two-body forces derivable from a potential energy $\hat{v}_{ij} = v(\underset{\sim}{r}_{ij})$ then the nuclear Hamiltonian is given by

$$\hat{H} = \sum_{i=j}^{A} \hat{t}_i + \sum_{j,i<j} \hat{v}_{ij}$$

where $\hat{t}_i = -\hbar^2\nabla_i^2/2m_i$. This procedure results in the HF equations

$$-\frac{\hbar^2}{2m}\nabla^2\phi_i(\underset{\sim}{r}) + \left[\int \rho(\underset{\sim}{r}')v(|\underset{\sim}{r}-\underset{\sim}{r}'|)d^3r'\right]\phi_i(\underset{\sim}{r}) \qquad (1.1)$$

$$-\int \rho(\underset{\sim}{r}',\underset{\sim}{r})v(|\underset{\sim}{r}-\underset{\sim}{r}'|)\phi_i(\underset{\sim}{r}')d^3r' = \varepsilon_i\phi_i(\underset{\sim}{r})$$

Here the one-body density matrix is defined by

$$\rho(\underset{\sim}{r},\underset{\sim}{r}') = \sum_{i=1}^{A} \phi_i^*(\underset{\sim}{r})\phi_i(\underset{\sim}{r}'), \text{ and } \rho(\underset{\sim}{r}) \equiv \rho(\underset{\sim}{r},\underset{\sim}{r}) = \Sigma|\phi(\underset{\sim}{r})|^2$$

is the local nucleon density at $\underset{\sim}{r}$.

The HF equations are solved by an iterative procedure: one begins with a 'reasonable' set $\{\phi_i\}$ and from them constructs the density matrix. This allows solution of the HF equations for a new set of ϕ_i and the corresponding eigenvalues ε_i. The process is repeated until it converges to a self-consistent solution. In eqn. (1.1) we identify the local direct and non-local exchange potential fields.

(iii) Density Matrix Expansion:

If one uses a finite range two-body interaction, the exact solution of the (integro-differential) HF equations (1.1) is time consuming. Hence, an approximation was devised by Negele and Vautherin, (NV 72), to simplify the numerical problems, essentially by approximating the exchange, or Fock term. This proceeds by deriving an approximate form of the off-diagonal density matrix $\rho(\underset{\sim}{r},\underset{\sim}{r}')$ as follows. Define the relative and center of mass co-ordinates of two nucleons at $\underset{\sim}{r}$, $\underset{\sim}{r}'$ as $\underset{\sim}{s} = \underset{\sim}{r}-\underset{\sim}{r}'$, $\underset{\sim}{R} = \frac{1}{2}(\underset{\sim}{r}+\underset{\sim}{r}')$, and also define

$$\rho(\underset{\sim}{R};\underset{\sim}{s}) = \rho(\underset{\sim}{R} + \tfrac{1}{2}\underset{\sim}{s},\underset{\sim}{R} - \tfrac{1}{2}\underset{\sim}{s}) = \rho(\underset{\sim}{r},\underset{\sim}{r}') \ .$$

Also, denote by $\hat{\rho}(\underset{\sim}{R};\underset{\sim}{s})$ the angle-average of the density matrix. $\hat{\rho}$ is actually a function of $\underset{\sim}{R}$ and $|\underset{\sim}{s}|$, being equal to $\rho(\underset{\sim}{R};\underset{\sim}{s})$ averaged over the directions $\Omega_{\underset{\sim}{s}}$ of $\underset{\sim}{s}$. Negele and Vautherin have

expanded $\hat{\rho}$ in powers of s. Their result is the DME

$$\hat{\rho}(\underset{\sim}{R};\underset{\sim}{s}) = \frac{1}{sk_F} \sum_{n=0}^{\infty} (4n+3) j_{2n+1}(sk_F) \left[Q_n\left(\left(\frac{\nabla_1 - \nabla_2}{2k_F} \right)^2 \right) \rho(\underset{\sim}{R}_1, \underset{\sim}{R}_2) \right]_{\underset{\sim}{R}_1 = \underset{\sim}{R}_2 = \underset{\sim}{R}} \tag{1.2}$$

$$= \frac{3}{sk_F} j_1(sk_F)\rho(\underset{\sim}{R}) + \frac{35}{2sk_F^3} j_3(sk_F) \left[\frac{1}{4}\nabla^2\rho(\underset{\sim}{R}) - \tau(\underset{\sim}{R}) + \frac{3}{5} k_F^2 \rho(\underset{\sim}{R}) \right] + O(s^4). \tag{1.3}$$

Here Q_n is defined in terms of the usual Legendre polynomial P by $Q_n(z^2) = (-1)^n P_{2n+1}(iz)/(iz)$, j_n are spherical Bessel functions, and

$$\tau(\underset{\sim}{R}) = \sum_{i=1}^{A} \nabla\phi_i^*(\underset{\sim}{R}) \cdot \nabla\phi_i(\underset{\sim}{R}) \tag{1.4}$$

is the so-called kinetic-energy-density.

One exploits the fact that the two-body force v(s) appearing in (1.1) has a short range by keeping only low powers of s in eqn. (1.3).

It bears mentioning that the parameter k_F which has been formally introduced in the right-hand side of (1.2) is completely arbitrary. However, if the expansion for $\hat{\rho}$ is truncated, as in (1.3), then the choice of k_F influences the approximation of $\hat{\rho}$.

The DME with k_F given by the LDA, eqn. (2.2), was used by Negele and Vautherin to approximate the potential energy density due to the two-body reaction matrix G. Its applicability has been widely discussed, (NV 72) (Spr+ 75) (BS 77).

(iv) Skyrme's Interaction:

The DME provides a satisfactory theoretical derivation for the form of Skyrme's interaction, because the DME-approximation potential energy density is in fact exact for the Skyrme force.

This model of the effective nucleon-nucleon interaction v(12) was originally suggested by Skyrme (Sky 56), (Sky 59), and recently revived by Vautherin and Brink, (VB 72), for the purpose of performing HF calculations. It is zero-range, momentum dependent, and contains a two-body spin-orbit force and a three-body force which is intended to describe many body effects phenomenologically. It can be written as a potential

$$V = \sum_{\substack{i,j \\ i<j}} v_{ij} + \sum_{\substack{i,j,k \\ i<j<k}} v_{ijk}$$

where typically:

$$v_{12} = t_0(1 + x_0 P_\sigma)\delta + \frac{1}{2} t_1(\delta k^2 + k'^2 \delta) + t_2 k'\cdot\delta k + iW(\underset{\sim}{\sigma}_1+\underset{\sim}{\sigma}_2)\cdot k' \times \delta k \qquad (1.5)$$

and

$$v_{123} = t_3\delta(\underset{\sim}{r}_{12})\delta(\underset{\sim}{r}_{23}) \ . \qquad (1.6)$$

For the purposes of HF calculations, v_{123} can be replaced by an equivalent density-dependent two-body interaction:

$$v_{12}^{(3)} = \frac{1}{6} t_3 \rho((\underset{\sim}{r}_1+\underset{\sim}{r}_2)/2)\delta(1+P_\sigma) \ . \qquad (1.7)$$

The notation is defined in Appendix A.

Details concerning the use of Skyrme's force in HF calculations of spherical nuclei are developed in (VB 72) as are two sets of parameters $(t_o, x_0, t_1, t_2, t_3, W)$ denoted SI, SII. Further sets SIII to SVI are developed by M. Beiner et al. (Bei+ 75).

The HF equations for Skyrme's force read

$$-\nabla\cdot\left(\frac{\hbar^2}{2m_q^*(\underset{\sim}{r})}\nabla\phi_i\right) + (U_q(\underset{\sim}{r}) - i\underset{\sim}{W}_q(\underset{\sim}{r})\cdot\nabla\times\underset{\sim}{\sigma})\phi_i = \varepsilon_i\phi_i \ . \qquad (1.8)$$

For an N=Z nucleus without Coulomb field the effective mass, potential and spin-orbit form factor are given respectively by

$$\frac{\hbar^2}{2m^*} \equiv \frac{\hbar^2}{2m} - B = \frac{\hbar^2}{2m} + \frac{3t_1+5t_2}{16}\rho$$

$$U = 3t_0\rho/4 + 3t_3\rho^2/16 + (3t_1+5t_2)\tau/16$$

$$+ (5t_2-9t_1)\nabla^2\rho/32 - 3W\nabla\cdot\underset{\sim}{J}/4$$

$$\underset{\sim}{W} = 3W\nabla\rho/4 + (t_1-t_2)\underset{\sim}{J}/16 \ .$$

Equation (1.8) differs from (1.1) in that the momentum dependence of v_{12} has introduced the position dependent effective mass $m^*(\underset{\sim}{r})$, and terms proportional to τ and $\nabla^2\rho$ in the potential.

The Skyrme force has many desirable features; these include:

(a) the energy density is an algebraic function of ρ, τ and the spin density

$$\underset{\sim}{J}(\underset{\sim}{r}) \equiv -i \sum_{i,\sigma,\sigma'} \phi_i^*(\underset{\sim}{r},\sigma,q)\nabla\phi_i(\underset{\sim}{r},\sigma',q) \times \langle\sigma|\underset{\sim}{\sigma}|\sigma'\rangle \ .$$

Hence the parameters can be interpreted physically. Some of their properties are discussed in (VB 72) and (Bei+ 75).

(b) Because the force is zero-range, the Fock exchange potential is local, and the HF equations (1.8) are purely differential, thus lending themselves to fast numerical solution.

(c) Calculations with the force reproduce many nuclear properties remarkably well over a wide range of nuclei, with only a few adjustable parameters. Examples include: binding energies, charge and mass radii, charge density, fission barriers.

(d) The force can be reliably extrapolated to investigate properties of nuclear matter.

A review of nuclear self-consistent calculations with effective interactions is to be found in (QF 78).

CHAPTER II

LOCAL FERMI MOMENTUM AND EFFECTIVE INTERACTIONS

In this chapter we recall how the LFM was introduced, and then suggest why it may be relevant to the subject of effective interactions.

We begin by considering a homogeneous system composed equally of neutrons and protons, and occupying an 'infinite' volume Ω. (This would be a symmetric form of nuclear matter in which $\rho_n = \rho_p = \frac{1}{2}\rho$.) In this case the single-particle states are plane waves $\phi_{\underset{\sim}{k}}(\underset{\sim}{r}) = \exp(i\underset{\sim}{k}\cdot\underset{\sim}{r})/\sqrt{\Omega}$, due to the translational symmetry. Consequently the one-body density matrix

$$\rho(\underset{\sim}{r},\underset{\sim}{r}') = \sum_{k<k_F} \phi^*_{\underset{\sim}{k}}(\underset{\sim}{r})\phi_{\underset{\sim}{k}}(\underset{\sim}{r}')$$

is given by (Sla 60):

$$\rho(\underset{\sim}{r},\underset{\sim}{r}') = \rho(\underset{\sim}{R};\underset{\sim}{s}) = \rho(\underset{\sim}{R})\ \frac{3}{sk_F}\ j_1(sk_F)$$

$$\equiv \rho\hat{j}_1(sk_F)\ , \qquad (2.1)$$

where in this infinite system the Fermi momentum k_F is related to the constant nucleon density ρ by

$$\rho = \frac{2}{3\pi^2}\ k_F^3 = \rho(\underset{\sim}{R})\ .$$

If, instead, we study a system of finite extent, (i.e. an atomic nucleus), in the independent-particle approximation, then

$$\rho(\underset{\sim}{r},\underset{\sim}{r}') = \sum_i \phi_i^*(\underset{\sim}{r})\phi_i(\underset{\sim}{r}')$$

where the sum is taken over occupied single-particle states i. A common approximation (BGW 58), (Neg 70) - the so-called Slater approximation - is to use plane waves for ϕ_i, with the Fermi momentum given by the Local Density Approximation:

$$k_F(\underset{\sim}{R}) = [\frac{3\pi^2}{2}\rho(\underset{\sim}{R})]^{1/3} . \qquad (2.2)$$

In this case one obtains the approximate Slater result

$$\rho(\underset{\sim}{R},\underset{\sim}{s}) \approx \rho(\underset{\sim}{R})\hat{j}_1(sk_F(\underset{\sim}{R})) \qquad (2.3)$$

It can be seen, by inspecting the DME (1.3) that there are corrections of order s^2 to the Slater approximation (2.3). In any event, the Slater approximation can be regarded as giving a prescription for mapping $\rho(\underset{\sim}{R};\underset{\sim}{s})$ from the infinite to the finite system; namely to retain the same form (2.1) but replace k_F by a function of $\rho(\underset{\sim}{R})$ (2.2).

A more recent suggestion, due to (CB 78) is called the LFM approximation. This involves retaining the Slater form (2.1) and replacing k_F with the LFM, defined:

$$\hat{k}(\underset{\sim}{R}) = [\frac{5}{3}(\tau(\underset{\sim}{R}) - \frac{1}{4}\nabla^2\rho(\underset{\sim}{R}))/\rho(\underset{\sim}{R})]^{1/2} . \qquad (2.4)$$

This choice causes the second term of (1.3) to vanish, and can be regarded as a modified DME

$$\rho(\underset{\sim}{R};\underset{\sim}{s}) = \rho(\underset{\sim}{R})\hat{j}_1(s\hat{k}(\underset{\sim}{R})) + O(s^4) \ , \qquad (2.5)$$

and has the advantage of being good to order s^4. This is an important advantage over the Slater approximation due to the short but finite range of the nuclear force. Consider for example, the successful results obtained by (NV 72) using the standard DME (eqn. (1.3) with k_F chosen by the LDA) which is also accurate to s^4. As yet, not as much effort has gone into the use of the Campi-Bouyssy modified DME (2.5). In the next chapter we will develop some observations in this connection.

Next, we turn to the subject of effective interactions.

In the Brueckner theory of nuclear matter (Day 67), one describes the two-body nucleon-nucleon interaction by the reaction matrix $\langle \underset{\sim}{k}' | G^{JT}_{LL'}(k_F, \underset{\sim}{K}, \cdots) | \underset{\sim}{k} \rangle$. It is not unusual to replace the complicated quantity G with an effective interaction $v_{eff}(k_F, r)$ which is meant to represent the two-body interaction in some average sense, (BGW 58) (Neg 70). If correctly constructed it is hoped that v_{eff} will contain enough information to reproduce the bulk properties of finite systems, when used with the appropriate calculational technique, (e.g. HF method). Examples of effective interactions are the density independent Brink and Boecker force B1 (BB 67), the density dependent force G-0 of Campi and Sprung, (CS 72), and Skyrme's interaction.

In this setting the LDA is also extensively used, because the G-matrix is calculated in nuclear matter, and the LDA pro-

vides a prescription for k_F in finite systems. Thus, one replaces k_F dependence in v_{eff} with (local) density dependence. In this way one obtains the re-arrangement energy (see eqn. (3.3)) which is crucial (SVE 79) to obtaining sufficient binding in finite nuclei with single-particle energies which are not too low. Also, one reproduces saturation properties of finite nuclei with the density dependent term phenomenologically accounting for many-body effects.

Given that the LFM $\hat{k}$ is a more accurate prescription for studying finite nuclei than is the LDA $k_F(\underset{\sim}{R})$, it seems natural to ask whether or not it is possible to construct an effective interaction with dependence upon $\hat{k}$; that is, upon τ and $\nabla^2\rho$ as well as ρ in a particular combination. That the interaction might depend on these quantities, in principle, is not unreasonable because they are independent in finite nuclei. In nuclear matter τ, ρ and k_F are all related (c.f. eqn. (5.2)) and $\nabla^2\rho = 0$, so that one could not distinguish between dependences on these various quantities in an infinite system. The investigation of the properties of a $\hat{k}$-dependent interaction is the subject of the next chapter.

CHAPTER III

INVESTIGATION OF INTERACTION DEPENDING ON $\hat{k}$

In this section we will consider an interaction of the Skyrme type, but with $V_{12}^{(3)}$ modified in that the density-dependence in eq. (1.7) is replaced with dependence on the LFM $\hat{k}$ raised to an exponent 2β. We intend to show that a force of this type will have zero rearrangement energy.

However, since the Skyrme force is momentum dependent, it is worthwhile to first investigate the origin of rearrangement energy in this case. We start with some definitions, which are valid in the case of a true Skyrme force. The total energy is given by

$$E_{tot} = \sum_{i=1}^{A} \langle i|p^2/2m|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\tilde{v}_{12}|ij\rangle + \frac{1}{6}\sum_{ijk}\langle ijk|\tilde{v}_{123}|ijk\rangle \tag{3.1}$$

$$= \int H(\underset{\sim}{r})d^3r$$

where the tilde denotes an antisymmetrized matrix element. The Hartree-Fock energy is defined

$$E_{HF} = \frac{1}{2}\sum_{j}(\varepsilon_i + t_i) \tag{3.2}$$

with ε_i the i^{th} single-particle energy and $t_i = \langle i|p^2/2m|i\rangle$.

From these, the rearrangement energy is defined

$$E_{REAR} = E_{TOT} - E_{HF} \ . \tag{3.3}$$

We also note the following two facts derived in (VB 72). First of all, for the Skyrme force $V_{123} = t_3\delta(\underset{\sim}{r}_{12})\delta(\underset{\sim}{r}_{13})$ which implies

$$\begin{aligned} \frac{1}{6} \sum_{ijk} \langle ijk|\tilde{v}_{123}|ijk\rangle &= \frac{1}{2} \sum_{ij} \langle ij|\tilde{v}^{(3)}_{12}|ij\rangle \\ &= \frac{1}{4} t_3 \int \rho_n\rho_p\rho \\ &= \int H_3 \ . \end{aligned} \tag{3.4}$$

Secondly it is shown that

$$\varepsilon_i = t_i + \sum_j \langle ij|\tilde{v}_{12}|ij\rangle + \frac{1}{2} \sum_{jk} \langle ijk|\tilde{v}_{123}|ijk\rangle \ .$$

Adding t_i to both sides of this equation, summing over i and dividing by 2, yields the HF energy:

$$\frac{1}{2} \sum_i (\varepsilon_i + t_i) = \sum_i t_i + \frac{1}{2} \sum_{ij} \langle ij|v_{12}|ij\rangle + \frac{1}{4} \sum_{ijk} \langle ijk|v_{123}|ijk\rangle \ .$$

Subtracting this from E_{TOT} (eqn. (3.1)) gives

$$\begin{aligned} E_{REAR} &= -\frac{1}{12} \sum_{ijk} \langle ijk|\tilde{v}_{123}|ijk\rangle \\ &= -\frac{1}{8} t_3 \int \rho_n\rho_p\rho \ , \end{aligned} \tag{3.5}$$

where (3.4) has been used.

Because the forces we will study are to be defined by a modified $v_{12}^{(3)}$, (with no corresponding v_{123} to be introduced), the above method of calculating the rearrangement energy will not be useful. However, the above serves as an explanation of the origin of rearrangement energy, as well as a useful check on the following alternate method for obtaining E_{REAR}.

Consider the single-particle equation (1.8) without the spin-orbit term:

$$-\frac{\hbar^2}{2m}\nabla^2\phi_i + \nabla\cdot(B\nabla\phi_i) + U_i\phi_i = \varepsilon_i\phi_i \ .$$

We multiply by ϕ_i^*, sum over i, and integrate over space,

$$\int \left(-\frac{\hbar^2}{2m}\phi_i^*\nabla^2\phi_i + \phi_i^*\nabla\cdot(B\nabla\phi_i) + U_i|\phi_i|^2\right) = \sum_i \varepsilon_i \int |\phi_i|^2 \ .$$

Integrating by parts

$$\int \left(\frac{\hbar^2}{2m}\tau - B\tau + \Sigma_i U_i|\phi_i|^2\right) = \Sigma_i \varepsilon_i \ .$$

Again, we add $\Sigma_i t_i$ and divide by 2

$$\int \frac{\hbar^2}{2m}\tau + \frac{1}{2}\int (-B\tau + \Sigma_i U_i|\phi_i|^2) = E_{HF} \ .$$

Then using the explicit forms of $-B = \hbar^2/2m^* - \hbar^2/2m$, U_i and

$H(\underset{\sim}{r}) = \hbar^2\tau(\underset{\sim}{r})/2m + \sum_{j=0}^{3} H_j(\underset{\sim}{r})$ from (VB 72) it is not hard to show that (3.6) becomes

$$\int (H + \frac{1}{8} t_3 \rho_n \rho_p \rho) = E_{HF}$$

which agrees with (3.5). (Here $H_j \sim t_j$.)

Thus the momentum dependent terms in Skyrme's interaction do not contribute to E_{REAR}; only the density-dependent term proportional to t_3 does so.

Now one is in a position to look at an interaction depending on the LFM $\hat{k}$. In analogy with the Skyrme force we will choose

$$v_{12}^{(3)} = \frac{1}{6} t_3 \hat{k}^{2\beta}((\underset{\sim}{r}_1+\underset{\sim}{r}_2)/2)\delta(\underset{\sim}{r}_{12})(1 + x_3 P_\sigma) \ . \qquad (3.7)$$

This will produce (see Appendix A) a contribution to the energy density H, of

$$H_3 = \frac{1}{24} t_3 \hat{k}^{2\beta}[(1-x_3)(\rho_n^2+\rho_p^2) + 4(1 + \frac{1}{2} x_3)\rho_n\rho_p] \hat{k}^{2\beta}\chi \ . \qquad (3.8)$$

Note that, since we no longer require the H_3 arising from $v_{12}^{(3)}(\hat{k})$ to agree with that arising from a v_{123}, (because no v_{123} has been introduced for this $\hat{k}$ force), we have introduced a new exchange parameter x_3, not necessarily equal to 1.

More generally, one need not restrict the $\hat{k}$ dependence of v_{eff} to be that given by (3.7). However, it suffices to consider this case, because the contribution to E_{REAR} caused by

the dependence of v_{eff} on $\hat{k}$ arises solely from the quantities ϕ_i^*, $\nabla\phi_i^*$, $\nabla^2\phi_i^*$ appearing in $\hat{k}$. This will be made clear in the following calculation, in which we show that this contribution vanishes identically.

The HF equations are the Euler-Lagrange equations derived by varying the ϕ_i^* so that $E_{TOT} = \int H$ is minimized. The modified H_3 (eqn. (3.8)) will introduce new terms into the HF equations, resulting from

(i) $\hat{k}^{2\beta} \frac{\partial \chi}{\partial \phi_i^*}$ (ordinary term),

(ii) $\chi \frac{\partial \hat{k}^{2\beta}}{\partial \mu}$ (rearrangement terms)

where $\mu \in \{\phi_i^*, \nabla\phi_i^*, \nabla^2\phi_i^*\}$.

Hence the single-particle equation reads

$$-\frac{\hbar^2}{2m}\nabla^2\phi_i + \frac{\partial H_3}{\partial \phi_i^*} - \nabla\cdot\frac{\partial H_3}{\partial \nabla\phi_i^*} + \nabla^2\frac{\partial H_3}{\partial \nabla^2\phi_i^*} + \nabla\cdot(B\nabla\phi_i) + U_i\phi_i = \varepsilon_i\phi_i \qquad (3.9)$$

where the terms B and U now arise only from the parameters t_0, t_1, t_2.

Recalling that

$$\hat{k}^2 = \frac{5}{3\rho}\left(\tau - \frac{1}{4}\nabla^2\rho\right) = \frac{5}{3\rho}\hat{\tau} \qquad (3.10)$$

$$= \frac{5}{3}\,\frac{-\frac{1}{4}\sum_j\left(\phi_j^*\nabla^2\phi_j - 2\nabla\phi_j^*\cdot\nabla\phi_j + \phi_j\nabla^2\phi_j^*\right)}{\sum_j \phi_j^*\phi_j},$$

we can calculate the three terms in (3.9) arising from H_3. Hence

$$\frac{\partial H_3}{\partial \phi_i^*} = \hat{k}^{2\beta} \frac{\partial \chi}{\partial \rho_i} \frac{\partial \rho_i}{\partial \phi_i^*} + \chi\beta\hat{k}^{2(\beta-1)} \frac{\partial \hat{k}^2}{\partial \phi_i^*}$$

$$= \hat{k}^{2\beta} \frac{\partial \chi}{\partial \rho_i} \phi_i + \frac{5}{3}\beta \frac{H_3}{\hat{k}^2} \left(-\frac{1}{4}\rho^{-1}\nabla^2\phi_i - \hat{\tau}\rho^{-2}\phi_i\right)$$

$$= \hat{k}^{2\beta} \frac{\partial \chi}{\partial \rho_i} \phi_i - X\left(\frac{1}{4}\nabla^2\phi_i + \frac{\hat{\tau}}{\rho}\phi_i\right)$$

where $X = 5\beta H_3/3\rho\hat{k}^2$, and ρ_i is ρ_p or ρ_n.

Similarly $$-\nabla \cdot \frac{\partial H_3}{\partial \nabla \phi_i^*} = -\nabla\cdot\left(X \frac{1}{2}\nabla\phi_i\right)$$

and $$\nabla^2 \frac{\partial H_3}{\partial \nabla^2 \phi_i^*} = -\frac{1}{4}\nabla^2(X\phi_i) .$$

If we put these results into (3.9), and perform as usual $\int \Sigma_i \phi_i^*$, then these new terms will produce:

$$\int \left[\hat{k}^{2\beta} \sum_i \frac{\partial \chi}{\partial \rho_i} |\phi_i|^2 - X\hat{\tau}\rho^{-1}\rho - \frac{1}{4}\sum_i \phi_i^*[X\nabla^2\phi_i + 2\nabla\cdot(X\nabla\phi_i) + \nabla^2(X\phi_i)]\right] ,$$

which upon integration by parts becomes

$$\int \left[\hat{k}^{2\beta} \sum_i \frac{\partial \chi}{\partial \rho_i} |\phi_i|^2 - X\hat{\tau} + X\left[-\frac{1}{4}\sum_i (\phi_i^*\nabla^2\phi_i - 2|\nabla\phi_i|^2 + \phi_i\nabla^2\phi_i^*)\right]\right]$$

$$= \int \hat{k}^{2\beta} \sum_i \frac{\partial \chi}{\partial \rho_i} |\phi_i|^2 . \qquad (3.11)$$

due to (3.10).

We show below that this final contribution just equals $2\int H_3$. Thus, the single-particle equation (3.9) has evolved into

$$\int \left(\frac{\hbar^2}{2m}\tau + 2H_3 + 2\sum_{j=0}^{2} H_j\right) = \Sigma_i \varepsilon_i \ ,$$

the first and third terms in the integral arising exactly as before. Adding $\Sigma_i t_i$ to this last equation, and dividing by two yields

$$\int H = \frac{1}{2}\sum_i (\varepsilon_i + t_i), \quad \text{or} \quad E_{TOT} = E_{HF} \ .$$

This completes the proof that for a $\hat{k}$ dependent force the rearrangement energy is exactly zero. (To show that (3.11) equals $2\int H_3$, it suffices by (3.8), to show that $\Sigma_i \frac{\partial \chi}{\partial \rho_i} |\phi_i|^2 = 2\chi$; but using the definition (3.8) of χ we have

$$\Sigma_i \frac{\partial \chi}{\partial \rho_i} |\phi_i|^2 = \frac{t_3}{24}\sum_i ((1-x_3)2\rho_i + 4(1+\tfrac{1}{2}x_3)\rho_{\bar{i}})|\phi_i|^2$$

$$= \frac{t_3}{24}\left(2(1-x_3)(\rho_n^2+\rho_p^2) + 4(1+\tfrac{1}{2}x_3)(\rho_n\rho_p+\rho_p\rho_n)\right)$$

$$= 2\chi \ .)$$

The feature of having zero rearrangement energy is rather undesirable. Its consequence is that, if the force is able to reproduce the binding energies of nuclei, then the single-particle energies must be very spread out. This phenomenon occurs for forces having a small effective mass,

$m^* << m$. To understand this qualitatively, one can use the Fermi-gas model of the nucleus to argue that the Fermi momentum k_F is fixed by A particles occuping a volume Ω. Then the average 'Hamiltonian' of a single particle at the Fermi surface can be written $\hbar^2 k_F^2/2m^* + U$. As m^* decreases, the effective kinetic energy increases; but the binding energy of the least bound particle (of momentum $\hbar k_F$) must be of the order of a few MeV. It follows that U must become deeper. Hence, ε_i becomes more negative and the level density decreases as m^* does. As an example, one interaction which has $E_{REAR} = 0$ is the Skyrme parametrization S-V, in which $t_3 = 0$, (Bei+ 75). It also has a low effective mass $m*/m \approx .38$. It is not surprising then to find the following relationship between a $\hat{k}$ dependent force and S-V. Consider (3.7) in the case $\beta = 1$ and $x_3 = -.5$. Then

$$H_3 = \frac{1}{12} t_3 \hat{k}^2 (\frac{3}{4} \rho^2 + 0) = \frac{1}{16} \frac{5}{3} t_3 (\tau - \frac{1}{4} \nabla^2 \rho) \rho \ .$$

But the energy density due to t_1 and t_2 also contains terms proportional to $\rho\tau$ and $\rho\nabla^2\rho$ (VB 72). Hence in this case the modified t_3 term can be absorbed into H_1 and H_2, and since there is no density dependence, this $\hat{k}$ force is essentially the same as the S-V force.

Because the $\hat{k}$ interaction is lacking in effective mass, and is similar to the S-V force which has been investigated elsewhere, we will modify our choice of interaction so that the rearrangement energy is non-zero. This will be done in the

next chapter.

Finally, we can make an observation regarding the use of the Campi-Bouyssy version of the DME approximation (eqn. (2.5)), as mentioned in the last chapter.

Consider, for example the force of (BB 67). Being independent of density, it too has no rearrangement energy in an exact HF calculation. If, however, one wishes to do a HF calculation using the Campi-Bouyssy DME approximation, one will obtain a potential energy density $V(r,\hat{k})$ which is a function of $\hat{k}$. Now as we have seen, the $\hat{k}$ dependence gives rise to no rearrangement energy, so that the Campi-Bouyssy DME (CB-DME) can be very accurate.

This is to be compared with the standard DME of (NV 72) with which one obtains $V(r,\rho)$. In principle then, one might expect the standard DME to give rise to a spurious rearrangement energy due to ρ.

However, since the standard and the CB-DME only differ in terms of order s^4, and the CB-DME gives rise to no rearrangement energy, one should also expect E_{REAR} to be very small for the standard DME. This provides a theoretical basis to explain the findings of (Spr+ 75) who obtained $E_{REAR} \approx 0$ in actual numerical calculations using the standard DME and the force of (BB 67).

Alternatively, if the interaction to be used is density dependent, this dependence remains when the CB-DME is used, re-

sulting in $V(r,\rho,\hat{k})$. Consequently such a force will provide a rearrangement energy, arising from the ρ dependence only.

In summary, insofar as one can neglect terms of order s^4, the use of either the standard- or the CB-DME approximations should give rise to no rearrangement energy additional to that resulting from the interaction with which one is concerned.

CHAPTER IV

CHOICE OF INTERACTION

In Chapter 2 it was suggested that the effective nuclear interaction in finite systems could in principle be a function of quantities such as τ and $\nabla^2\rho$, as well as of ρ. In the previous chapter we showed that if the interaction depended on $\hat{k}^2 \sim (\tau - \frac{1}{4}\nabla^2\rho)/\rho$ only, then it would lead to zero re-arrangement energy. Hence we suggest that in general one should choose the interaction to depend both on ρ and on $\hat{k}^2$.

Because we would like to continue, as much as possible, to investigate the LFM prescription, we have chosen to develop a force which depends on

$$\rho\cdot\hat{k}^2 \sim \tau - \frac{1}{2}\nabla^2\rho = \hat{\tau}$$

raised to a power β.

As a model of this kind we use a modified Skyrme force, in which (1.7) is replaced by

$$v_{12}^{(3)} = \frac{1}{6}\bar{t}_3\hat{\tau}^{\beta}((\underset{\sim}{r}_1+\underset{\sim}{r}_2)/2)\delta(\underset{\sim}{r}_{12})(1 + x_3P_\sigma) \ . \qquad (4.1)$$

This can be considered as a force having a kinetic-energy-density dependent saturation term. For the interaction (4.1) to be meaningful, it is necessary that $\hat{\tau}$ be positive if β is non-integral. Whereas $\tau = \Sigma_i|\nabla\phi_i|^2$ is necessarily positive,

$-\frac{1}{4}\nabla^2\rho$ can be negative; in particular it must be so in the nuclear exterior. We also note that the true-kinetic-energy-density $\Sigma_i \phi_i^* \nabla^2 \phi_i \equiv \tau' = \tau - \frac{1}{2}\nabla^2\rho = \hat{\tau} - \frac{1}{4}\nabla^2\rho$ (for a spherical or time-reversal invariant system, c.f. eqn. (28) of (VB 72)) is negative in the exterior. These points notwithstanding, in actual numerical calculations $\hat{\tau}$ did prove to remain positive for all $0 \leq r < \infty$, and its sign therefore presented no difficulty in practice.

It will now be shown that a force with $v_{12}^{(3)}$ of eqn. (4.1) possesses a rearrangement energy. The energy density due to (4.1) is

$$H_3 = \frac{1}{24}\bar{t}_3 \hat{\tau}^\beta [(1-x_3)(\rho_n^2+\rho_p^2) + 4(1+\tfrac{1}{2}x_3)\rho_n\rho_p] \qquad (4.2)$$

$$\equiv \hat{\tau}^\beta \chi \ ,$$

similar to (3.8). From the previous evaluation of $E_{REAR} = 0$ for the $\hat{k}$ dependent force (3.7), it is clear that due to (4.2):

$$\dot{E}_{REAR} = -\frac{1}{2}\int \Sigma_i \phi_i^* [X \frac{\partial \hat{\tau}}{\partial \phi_i^*} - \nabla\cdot(X \frac{\partial \hat{\tau}}{\partial \nabla \phi_i^*}) + \nabla^2(X \frac{\partial \hat{\tau}}{\partial \nabla^2 \phi_i^*})] \ . \qquad (4.3)$$

Here $X \equiv \partial H_3/\partial\hat{\tau} = \beta\hat{\tau}^{\beta-1}\chi = \beta H_3/\hat{\tau}$. The three factors in (4.3) involving $\hat{\tau}$ are (from (3.10)):

$$\frac{\partial \hat{\tau}}{\partial \phi_i^*} = -\frac{1}{4}\nabla^2\phi_i \ , \quad \frac{\partial \hat{\tau}}{\partial \nabla \phi_i^*} = \frac{1}{2}\nabla\phi_i \ , \quad \frac{\partial \hat{\tau}}{\partial \nabla^2 \phi_i^*} = -\frac{1}{4}\phi_i \ .$$

Substituting into (4.3) and integrating by parts yields

$$E_{REAR} = -\frac{1}{2}\int X\,\Sigma_i - \frac{1}{4}\,(\phi_i^*\nabla^2\phi_i - 2\nabla\phi_i^*\cdot\nabla\phi_i + \phi_i\nabla^2\phi_i^*)$$

$$= -\frac{1}{2}\int (\beta H_3/\hat{\tau})\,\hat{\tau}$$

$$= -(\beta/2)\int H_3 \,. \qquad (4.4)$$

Consequently $E_{REAR} \neq 0$ unless $\beta = 0$ or $\bar{t}_3 = 0$; in either of these uninteresting cases the interaction is equivalent to S-V.

Thus a modified Skyrme-type force - with $t_3 = 0$ and $v_{12}^{(3)}$ given by (4.1) was used to perform DME-HF calculations for doubly closed shell spherical nuclei. It should be noted, again, that the DME is exact for this type of force. The complete form of the interaction is defined in Appendix A, along with some details concerning the method of calculation.

Before presenting the results obtained, some discussion concerning the choice of parameters of the force is in order. The available parameters are:

β	-	exponent of $\hat{\tau}$
$t_0\ t_1\ t_2\ \bar{t}_3$	-	'well' strengths
$x_0\ x_1\ x_2\ x_3$	-	exchange factors
W	-	spin-orbit strength.

We have in particular investigated the case $\beta = 1/10$ for the following reason. There exist several successful effective in-

teractions (CS 72), (KTB 80) with density dependent terms varying as $\rho^{1/6}$. Now in nuclear matter one has $\hat{\tau} = \tau \sim k_F^5$, while $\rho \sim k_F^3$. Hence $\rho^\gamma \sim \hat{\tau}^{3\gamma/5}$, so that $\rho^{1/6}$ corresponds to $\hat{\tau}^{1/10}$. Of course in finite nuclei ρ and τ are not so simply related, but this argument serves as a rough guide, insofar as we can consider the interior regions of the nucleus as a portion of nuclear matter. One could also appeal to the Thomas-Fermi approximation for justification. In addition to using $\beta = 1/10$ we have also used $\beta = 1$, that is a force without exponent.

The strengths t_0, t_1, t_2, $\bar{t}_3$ were also chosen using nuclear matter as a guide. More is said about this in the next chapter, where the nuclear matter properties of the force are studied. Generally $t_0 < 0$; $t_1, t_3 > 0$.

The spin exchange parameters $x_i (i = 0, \cdots, 3)$ were introduced into the potential $v_{12} + v_{12}^{(3)}$ in factors $(1 + x_i P_\sigma)$ multiplying t_i. Consider for instance $i = 2$: this is a p-wave interaction term (because its matrix elements are proportional to $|\nabla\phi(0)|^2$) and is repulsive in nuclear matter if $t_2 > 0$ (see eqn. (5.3)). In (BS 71) several realistic potentials were found to have both ^3P and ^1P interactions repulsive, the singlet being stronger. This would occur for the present force if, when $t_2 > 0$, $1 + x_2 P_\sigma$ were larger in the singlet case. But $P_\sigma = +1, (-1)$ for triplet, (singlet), so that $-1 < x_2 < 0$ would be ideal. In the various Skyrme parametrizations, t_2 is actually

found to have either sign, and is always smaller than t_1.

The parameter x_0 affects $\Delta \equiv r_n - r_p$, the difference between the neutron and proton RMS mass radii. This can be understood as follows. x_0 occurs in an s-wave interaction, as $t_0(1 + x_0 P_\sigma) = t_0(1 \pm x_0)$ according as the force acts between unlike/like nucleons provided the unlike pair are in the antisymmetric isospin state. As $t_0 < 0$ this term will be more attractive between like particles if $x_0 < 0$. In a nucleus with $N > Z$, there are more neutrons to bind with other neutrons, than protons with other protons. It follows that the neutrons will be more strongly bound than protons if $x_0 << 0$. This would cause $r_n < r_p$, contrary to experiment, and places a practical limit on x_0.

The spin orbit strength W in various Skyrme-like forces is found to vary from about 90 to 150 MeV fm^5. For the present forces, values near the upper end of this range were found to be necessary in order to adjust the binding energies of zirconium-90 and lead-208. We did not choose W to fit exactly the experimental splittings of the $p_{1/2}$, $p_{3/2}$ levels in oxygen-16.

For the cases $\beta = 1$ and $\beta = 1/10$, parameter sets (denoted TA and TX respectively) were adjusted to obtain good fits to the experimental binding energies B, and RMS charge radii r_{ch}, of the four doubly magic nuclei ^{16}O, ^{40}Ca, ^{90}Zr, ^{208}Pb. The parameter sets are defined in table I, and the results obtained

with them are given in table II. A more complete discussion of these two preliminary forces must occur in the next chapter.

TABLE I

Parameter	FORCE TA	FORCE TX
β	1	0.1
t_0 (MeV fm^3)	-1228.43	-1659.32
t_1 (MeV fm^5)	917.765	902.823
t_2 (MeV fm^5)	43.936	29.709
$\bar{t}_3$ (MeV fm$^{5\beta+3}$)	2331.93	3698.44
W (MeV fm^5)	162.0	167.9
x_0	.0046	-.0020
x_1, x_2, x_3	0.	0.

Definition of the parameter sets TA and TB introduced in Chapter IV.

TABLE IIa

Nucleus	Exp.[e] B/A	TA B/A	TA $-E_{REAR}$	TX B/A	TX $-E_{REAR}$
^{16}O	7.9760	7.9761	0.666	7.9806	0.848
^{40}Ca	8.5515	8.5560	0.854	8.5554	0.980
^{48}Ca	8.6669	8.6914	0.899	8.7016	1.007
^{56}Ni	8.6430	8.5668	0.975	8.5736	1.072
^{90}Zr	8.7102	8.7097	0.993	8.7102	1.080
^{132}Sn	8.3540	8.3569	0.983	8.3678	1.069
^{140}Ce	8.3764	8.4053	0.996	8.3758	1.092
^{208}Pb	7.8677	7.8676	1.01	7.8677	1.10

Reference: e = (WB 77)

Rearrangement and binding energies ($B = -E_{TOT}$) calculated with TX are compared with experimental binding energies. All values in MeV.

TABLE IIb

Nucleus	Radius	Exp	TA	TX
^{16}O	ch	2.73[a]	2.692	2.713
	n		2.630	2.651
	p		2.651	2.673
^{40}Ca	ch	3.48[f]	3.479	3.485
	n		3.384	3.389
	p		3.426	3.433
^{48}Ca	ch	3.48[f,g]	3.491	3.488
	n		3.663	3.657
	p		3.456	3.454
^{56}Ni	ch	3.75[d]	3.800	3.790
	n		3.697	3.684
	p		3.745	3.735
^{90}Zr	ch	4.27[c]	4.298	4.285
	n		4.365	4.348
	p		4.261	4.247
^{132}Sn	ch		4.749	4.730
	n		5.022	4.997
	p		4.711	4.692
^{140}Ce	ch		4.912	4.900
	n		5.060	5.042
	p		4.880	4.868
^{208}Pb	ch	5.50[b]	5.545	5.522
	n		5.765	5.734
	p		5.510	5.487

References: a = (SM 70) , b = (Fro+ 77) , c = (Faj+ 71)
d = (Bei+ 75) , f = (Sic+ 78) , g = (Woh+ 78)

RMS radii of the charge (ch), neutron (n) and proton (p) densities calculated with TA, TX, are compared with experimental RMS charge radii. All values in fm.

CHAPTER V

NUCLEAR MATTER PROPERTIES OF THE INTERACTION

In the two previous chapters, two preliminary parametrizations of the $\hat{\tau}^{\beta}$ dependent interaction were introduced. In this chapter we will derive the nuclear matter properties of the interaction, and use these to develop a preferred parametrization. To do this we will refer to the results for the energy density and single-particle equations for this force, which are developed in appendix A. We begin with some simple, though important, definitions.

Nuclear matter (NM) is an infinite, homogeneous, three-dimensional system of nucleons, interacting only through the nuclear force. In general, the neutron and proton densities ρ_n and ρ_p need not be equal. However, one usually considers symmetric NM in which $\rho_n = \rho_p$. An exception to this occurs when calculating the symmetry energy co-efficients, (to be defined later).

Along with ρ_n and ρ_p, other useful quantities are introduced as follows (q = n or p):

$$\begin{aligned} \rho_q &= k_{Fq}^3/3\pi^2 \quad , \quad \rho = \rho_n + \rho_p = 2k_F^3/3\pi^2 \\ \tau_q &= k_{Fq}^5/5\pi^2 \quad , \quad \tau = \tau_n + \tau_p \ . \end{aligned} \tag{5.1}$$

Note that $\tau \neq 2k_F^5/5\pi^2$ if $\rho_n \neq \rho_p$. In the symmetric case

$$\rho_n = \rho_p = \rho/2 \quad , \quad \tau_n = \tau_p = \tau/2 \quad , \quad k_{Fn} = k_{Fp}$$
$$\tau = 2k_F^5/5\pi^2 = 3\rho k_F^2/5 \tag{5.2}$$

and the only free parameter is ρ, or equivalently k_F.

For the $\hat{\tau}^\beta$ dependent effective interaction defined in appendix A, we will now derive the following three symmetric NM properties: (i) average energy per particle E_{NM}, (ii) compression modulus K, (iii) effective mass m*/m, and also (iv) symmetry energy co-efficient ε_1.

(i) Calculation of $E_{NM} < 0$

As $E_{NM} = H_{NM}/\rho$ is the average energy per particle, we use equations (A-4), (A-5) for the energy density H. In (symmetric) NM we set $\rho_n = \rho_p$, $\nabla^2\rho = 0$, $e^2 = 0$, $\hat{\tau} = \tau$, $\underset{\sim}{J} = \underset{\sim}{0}$. Simple algebra then yields

$$E_{NM} = T_S + \frac{3}{80}\,(3t_1+(5+4x_2)t_2)\rho k_F^2 + \frac{3}{8}\,t_0\rho + \frac{1}{16}\,\bar{t}_3\tau^\beta\rho \tag{5.3}$$

where $T_S = 0.6\,\hbar^2k_F^2/2m$ is the average kinetic energy per particle.

(ii) Compression modulus K > 0

This is defined by $K = k_F^2\partial^2E_{NM}/\partial k_F^2$ evaluated at the saturation Fermi momentum k_F which satisfies the saturation condition $\partial E_{NM}/\partial k_F = 0$. Remembering the dependence of T_S, ρ, τ on k_F this reads

$$0 = 2T_S + \frac{3}{16}\,(3t_1+(5+4x_2)t_2)\rho k_F^2 + \frac{9}{8}\,t_0\rho + \frac{1}{16}\,\bar{t}_3(5\beta+3)\tau^\beta\rho \ , \tag{5.4}$$

while K is given by

$$K = 2T_S + \frac{3}{4}\,(3t_1+(5+4x_2)t_2)\rho k_F^2 + \frac{9}{4}\,t_0\rho + \frac{1}{16}\,\bar{t}_3\,(5\beta+3)(5\beta+2)\tau^\beta\rho. \quad (5.5)$$

Before continuing with m*/m, it is worth remarking that eqns. (5.3), (5.4), (5.5) proved to be useful in searching for parameters. Specifically, they can be regarded as a system of three equations in the three quantities $3t_1 + (5+4x_2)t_2$, t_0 and $\bar{t}_3$. As such they can be inverted to yield:

$$t_0 = \frac{4(-3(5\beta+1)T_S + 5(5\beta+3)E_{NM} + K)}{15\beta\rho} \quad (5.6)$$

$$\bar{t}_3 = \frac{16(-3T_S + 15E_{NM} + K)}{5\beta\rho\tau^\beta(5\beta-2)}$$

$$3t_1+(5+4x_2)t_2 = \frac{40((5\beta+1)T_S-3(5\beta+3)E_{NM} - K)}{3\rho k_F^2(5\beta-2)}\,.$$

One can regard E_{NM}, K, k_F to be approximately known from experiment. For example the semi-empirical mass formula (MS 74) gives $E_{NM} \approx -16$ MeV and $K \approx 240$ MeV; giant monopole resonance frequencies indicate $K \approx 210 \pm 30$ MeV, and from extrapolated central densities of nuclei one finds $k_F \approx 1.35 \pm .07$ fm at saturation, (Bla 80) (Tre+ 81). Although K has not yet been determined unambiguously (FV 81), (Bue+ 81), a value considerably below 300 MeV does seem to be in order.

In practice then, one chooses β and usually sets all exchange parameters $x_i = 0$ to reduce the number of parameters. With reasonable values of E_{NM}, K, k_F, (5.6) then yields an

initial set of parameters. If these parameters give undesirable results for finite nuclei, they can be adjusted by using a new set of E_{NM}, K, k_F. In this way physical insight can guide the choice of parameters.

Equation (5.6c) only specifies the combination $3t_1+5t_2$, (if $x_2 = 0$). This raises the question of how to choose a particular value of t_1 and t_2. The answer lies in the fact that these parameters have a more pronounced effect on the calculated binding energy of small nuclei than on larger ones. This can be understood from (A-5), whereby for an N = Z nucleus with no Coulomb field

$$H_1+H_2 = (3t_1+5t_2)\rho\tau/16+(9t_1-5t_2)|\nabla\rho|^2/64 \ . \qquad (5.7)$$

By (5.6c) the first term is fixed. Now if t_1 increases, t_2 must decrease, and so the second term of (5.7) increases, causing E_{TOT} to increase. Furthermore, $|\nabla\rho|$ is appreciably different from zero only in the nuclear surface. Hence for small nuclei, which are almost all surface, a change in t_1 has the largest effect on E_{TOT}, and requiring that four doubly magic nuclei of widely varying size be properly bound restricts the choice of t_1.

We now continue with the nuclear matter properties.

(iii) Effective mass m*/m

This is obtained from (A-7) by setting $\rho_n = \rho_p$, yielding

$$\frac{m^*}{m} = \left[1 + \frac{\rho m}{8\hbar^2}\left(3t_1+(5+4x_2)t_2+\bar{t}_3\beta\rho\tau^{\beta-1}\right)\right]^{-1} . \qquad (5.8)$$

The effective mass can also be expressed in terms of the other NM properties by using (5.6) to replace the t_i parameters in (5.8). After some straightforward but tedious algebra, one obtains (using $\hbar^2/m = 41.47$ MeV fm^2) in the case $\beta = 0.1$ the result

$$\frac{m^*}{m} = \left(.9 + \frac{.1206\ E_{NM} + .01608\ K}{k_F^2}\right)^{-1} , \qquad (5.9)$$

and in the case $\beta = 1$:

$$\frac{m^*}{m} = \left(1.8 - \frac{.2411\ E_{NM} + .008038\ K}{k_F^2}\right)^{-1} . \qquad (5.10)$$

The effective mass near nuclear density is suggested by nucleon-nucleus scattering experiments to be roughly 0.7, (JLM 76).

(iv) Symmetry energy co-efficient ε_1

This quantity is defined, by considering non-symmetric NM, as follows:

$$E_{NM}(\alpha) = E_{NM}(0) + \varepsilon_1\alpha^2 + O(\alpha^4) , \qquad (5.11)$$

where $\alpha \equiv (\rho_n-\rho_p)/\rho$. Only even powers of α appear in the expansion (5.11) because neutrons and protons are treated symmetrically in NM - for example there is no Coulomb force.

The expression for ε_1 for a Skyrme force is given in

equation (37) of (VB 72). To obtain ε_1 for the present force one must set their $t_3 = 0$ and then include the effects of terms proportional to x_1, x_2, $\bar{t}_3$. These new contributions are derived in appendix B, so that the final result is

$$\varepsilon_1 = \frac{5}{9} T_S - \frac{1}{4} t_0 (x_0 + \frac{1}{2}) \rho - \frac{1}{8} x_1 t_1 \rho k_F^2 + \frac{1}{6} t_2 (1 + \frac{5}{4} x_2) \rho k_F^2 \qquad (5.12)$$

$$- \frac{1}{48} \bar{t}_3 (1+2x_3 - \frac{5}{3} \beta) \rho \tau^\beta .$$

This shows that x_0 should only affect the energy of nuclei with $N \neq Z$, insofar as $\rho_n \doteq \rho_p$ otherwise. The value of ε_1 can be estimated from the semiempirical mass formula to be about 30±5 MeV.

The NM properties of the two forces TA and TZ developed in the last chapter are given in table III. We see that E_{NM}, k_F and ε_1 fall into the experimental ranges mentioned above. However the values of K obtained from these forces are larger than the experimental upper limit of 240 MeV. It is well known that for Skyrme forces, values of K below 300 MeV are not consistent with obtaining proper binding, as discussed in (Bei+ 75). This is also true for our $\hat{\tau}^\beta$ force when $\beta = 1 > .4$. To see this, consider equation (5.6b) for $\bar{t}_3$. One requires $\bar{t}_3 > 0$ and $\beta > 0$ for the force to be physically reasonable. But $\beta > .4$ implies $5\beta - 2 > 0$, so that for $\bar{t}_3 > 0$, eqn. (5.6) requires that

$$- 3T_S + 15 E_{NM} + K > 0. \qquad (5.13)$$

Hence

$$K_{min} = 3T_S - 15\, E_{NM}$$

$$\approx 3(20) - 15(-16) = 300 \text{ MeV} .$$

Alternatively, if $\beta < .4$ the sense of the inequality in (5.13) changes and we see that $K < 300$ MeV is required. This has in fact been realized in the force TX where $\beta = 0.1$.

For both the forces TA and TX we also find that m^*/m is about .4 and that the re-arrangement energy is small (Table II). We previously rejected the $\hat{k}^2$-dependent force (3.7) because it has $E_{REAR} = 0$, and consequently a small effective mass like SV.

Fortunately, it is possible to remedy both the large K and low m^*/m problems of the preliminary forces, simultaneously. From (5.9), which holds for $\beta = 0.1$, we see that if K decreases, then m^*/m increases. Also if we fix $\beta = 0.1$ in (5.6b) the denominator will be negative, so that as K decreases $\bar{t}_3$ increases. This is reasonable because $E_{REAR} \sim \bar{t}_3$, and $|E_{REAR}|$ and m^*/m increase together. A similar argument, this time for the case $\beta = 1$ and using (5.10), shows that as K increases m^*/m increases.

It was thus desirable to develop three further parameter sets (denoted TB, TY, TZ) which have effective masses larger than 0.4. These parametrizations are defined in Table IV and results of HF calculations with them are presented in Table

V. Their NM properties are listed in Table VI.

These forces will be discussed in the next chapter, where set TY will be chosen as the preferred interaction of the $\hat{\tau}^{\beta}$ type.

TABLE III

NM Property	TA	TX
k_F (fm^{-1})	1.290	1.306
E_{NM} (MeV)	-16.133	-16.065
K (MeV)	350.0	283.0
m*/m	.4086	.4107
ε_1 (MeV)	36.42	34.69

The NM properties, which are defined in chapter V, of interactions TA, TX.

TABLE IV

	FORCE		
Parameter	TB	TY	TZ
β	1	0.1	0.1
t_0	-1014.18	-2365.45	-2844.26
t_1	448.681	603.878	407.12
t_2	-150.485	-115.585	-214.33
$\bar{t}_3$	9829.975	10812.45	15617.28
W	128.6	154.6	144.0
x_0	.24445	.0657	.0917
x_1, x_2, x_3	0.	0.	0.

Definition of the parameter sets TB, TY, TZ introduced in chapter V. Units are the same as in Table I.

TABLE Va

Nucleus	Exp. B/A	TB B/A	TB $-E_{REAR}$	TY B/A	TY $-E_{REAR}$	TZ B/A	TZ $-E_{REAR}$
^{16}O	7.9760	7.9754	2.807	7.9757	2.299	7.9750	3.213
^{40}Ca	8.5515	8.5469	3.449	8.5539	2.740	8.5524	3.907
^{48}Ca	8.6669	8.6793	3.639	8.6888	2.873	8.6740	4.144
^{56}Ni	8.6430	8.6247	3.881	8.5975	3.060	8.5971	4.435
^{90}Zr	8.7102	8.7099	3.940	8.7101	3.098	8.7056	4.500
^{132}Sn	8.3540	8.3403	3.957	8.3607	3.113	8.3563	4.571
^{140}Ce	8.3764	8.4345	4.018	8.3446	3.142	8.3224	4.573
^{208}Pb	7.8677	7.8676	4.070	7.8678	3.198	7.8695	4.698

Rearrangement and binding energies calculated with TB, TY, TZ are compared with experimental (WB 77) binding energies. All values are in MeV.

TABLE Vb

Nucleus	Exp	TB	TY	TZ
^{16}O	2.73	2.651	2.734	2.754
		2.589	2.674	2.695
		2.608	2.696	2.717
^{40}Ca	3.48	3.455	3.490	3.497
		3.363	3.394	3.399
		3.402	3.483	3.444
^{48}Ca	3.48	3.485	3.488	3.488
		3.643	3.644	3.637
		3.451	3.453	3.453
^{56}Ni	3.75	3.790	3.773	3.761
		3.690	3.666	3.653
		3.734	3.717	3.705
^{90}Zr	4.27	4.300	4.270	4.261
		4.360	4.325	4.307
		4.263	4.233	4.223
^{132}Sn		4.769	4.711	4.693
		5.012	4.954	4.916
		4.731	4.673	4.655
^{140}Ce		4.923	4.889	4.878
		5.048	5.008	4.981
		4.891	4.856	4.845
^{208}Pb	5.50	5.570	5.497	5.475
		5.760	5.680	5.636
		5.534	5.461	5.439

RMS radii of charge-, neutron- and proton-densities (from top to bottom) calculated with TB, TY, TZ are compared with experimental RMS charge radii. All values in fm. All references same as for table IIb.

TABLE VI

NM Property	TB	TY	TZ
k_F (fm^{-1})	1.275	1.326	1.345
E_{NM} (MeV)	-16.210	-16.072	-16.102
K (MeV)	480.0	240.0	207.8
m*/m	.5461	.5020	.5974
ϵ_1 (MeV)	34.56	30.35	26.77

The NM properties of interactions TB, TY, TZ.

CHAPTER VI

DISCUSSION OF RESULTS

In the previous chapter parametrizations TB, TY and TZ of the $\hat{\tau}^{\beta}$ dependent interaction were developed in order to obtain an effective mass considerably larger than .40, and the consequent increase in rearrangement energy. From table V we see that these forces indeed have considerable E_{REAR} contributions to E_{TOT}. This shows that in these forces the effect of the term of interest (eqn. (4.1)) is very substantial.

In the case of TB where $\beta = 1$, raising m* required using K = 480 MeV, which is very large. We see that TB gives the poorest overall fit to the experimental charge radii of all the five forces. In the case of TZ ($\beta = .1$) the more reasonable value of K = 208 MeV was obtained. Raising m*/m much beyond .60 when $\beta = .1$ would require lowering K even further (now going away from its experimental range) and would result in numerical difficulties in the solution of the HF problem. This would occur because as $\bar{t}_3$ increases, the contribution $-\frac{1}{4} V^2(\partial H_3/\partial \hat{\tau})$ to U_q increases (see (A-7)). This causes a 'feedback' of limited accuracy into the potential, because this term involves the fourth derivatives of the single-particle functions ϕ_i, which are calculated on a finite grid by a fourth order Runge-Kutta routine which integrates the HF equations (A-9).

Comparing the $\beta = .1$ forces TX and TZ we see that for TX the radii of the smaller nuclei are too small, and for the larger are too large, whereas for TZ the opposite is true. This motivated the development of parameter set TY which has values of K and m^*/m intermediate between those of TX, TZ and reproduces the experimental r_{ch} of all the nuclei exceptionally well. This also indicates that if one tried to increase m^*/m beyond .60 for this value of β, that such a force would have discrepancies in r_{ch} of the same type as those of force TZ, but of even larger magnitude.

Hence, on the basis of its reasonable NM properties, and its superior fit to the experimental binding energies and RMS charge radii of finite nuclei, we will refer to the parameter set TY as our preferred interaction. We shall now present the results obtained with this force in greater detail.

In figure 1 the total densities $\rho(r)$ calculated for ^{16}O, ^{40}Ca, ^{90}Zr, ^{208}Pb are compared with the force's symmetric NM density .157 fm^{-3}. In figures 2, 3 the separate neutron and proton contributions to $\rho(r)$ for ^{40}Ca and ^{208}Pb respectively, are graphed. In these figures, there are small oscillations of the density in the nuclear interior, which are typical of HF calculations.

In figures 4, 5 the charge densities of ^{40}Ca, ^{208}Pb calculated with the preferred interaction TY are compared with those of Skyrme III and with experiment. All calculated charge

densities include corrections (Ber+ 72) to account for the proton and neutron charge form factors, the electromagnetic spin-orbit force, and the nuclear center of mass motion. The experimental charge densities are accurate to within ± 1%. In the case of ^{40}Ca (fig. 4) the present force is seen to give a better fit to experiment than S III, particularly in the interior. In fact scaling the S III distribution to increase its RMS radius of 3.46 fm to the experimental value 3.48 fm would make its fit even poorer. In the case of ^{208}Pb (fig. 5) the charge density of force TY is also seen to follow the experimental results more closely than does the charge density of SIII, except for the central bump which extends to about 1.5 fm. This bump, which is associated with the shell structure of 3s protons (cf. fig. 3), is again typical of all HF calculations, and so should not be used to distinguish between the present force and S III. In this case scaling the S III density to reduce its RMS radius of 5.56 fm to the experimental value of 5.50 fm would improve its fit, but it would still be poorer in the surface region.

Also of interest are the single-particle energies ε_i of the force, which can be roughly compared with the experimental removal energies of a nucleon from the i^{th} level. These quantities are listed in table VII. We see that the orders of levels generally agree, and that the calculated level density is slightly lower. This is a common failing of HF calculations,

(CS 72). By comparison the deepest levels calculated with the force TZ which has m*/m = .60 lie about 12% higher than those of force TX.

The calculated 1p levels in ^{16}O are split by a larger amount than the experimental levels because of the value W = 155 MeV fm^5 that was required to fit the binding energies. These splittings for all five forces are compared in table VIII.

Because the modified ($\bar{t}_3$) term of our force contributes to the effective mass (A-7a), and hence to the nonlocality of the HF potential, it is worth examining m*/m and U. These quantities as calculated with the preferred interaction for ^{40}Ca and ^{208}Pb have been graphed in figures 6 and 7. We notice that m*/m has a strong radial dependence and approaches its nuclear matter value of .50 in the nuclear interior of lead. Despite the different nature of the present force, the curves in figs. 6, 7 have shapes very similar to those obtained with Skyrme II and presented in (VB 72).

Because our interaction depends on $\hat{\tau}$, it is of interest to look at the distributions of $\hat{\tau}$, τ_n and τ_p. These quantities as calculated in ^{40}Ca, ^{208}Pb are compared with Skyrme IV in figures 8, 9. Skyrme IV has approximately the same effective mass as TY. The similarity of the curves in these figures is also evident.

Finally, it is interesting to compare the quantities ρ and $\hat{\tau}$ which have been used to saturate the Skyrme and the present forces, Figures 10, 11 (for ^{40}Ca, ^{208}Pb) show $\hat{\tau}$ along

with τ and $f(\rho) \equiv .6\,(3\pi^2/2)^{2/3}\rho^{5/3}$, which equals τ and $\hat{\tau}$ in nuclear matter, as obtained with force TY. In both figures $f(\rho)$ has a steeper slope than does $\hat{\tau}$ or τ in the surface region. We also notice that $\hat{\tau}$ is smoother than τ in the surface. In the case of the large nucleus ^{208}Pb (fig. 11) the three curves agree quite closely in the nuclear interior, which they do not do in ^{40}Ca (fig. 10). In fig. 11 the interior oscillations of $\hat{\tau}$ and τ are out of phase with those of ρ, and those of $\hat{\tau}$ have the smallest magnitude.

The results of the preferred interaction presented in this chapter show that its properties concerned with finite nuclei in the HF approximation are in general not significantly different from those of the Skyrme forces. The agreement with experimental quantities is equally good for the two types of force. In addition we have seen in chapter V that our force TY possesses reasonable NM properties.

Hence we have successfully achieved the objective of Chapter IV, of developing an effective nuclear interaction with dependence on $\rho\hat{k}^2 \sim \hat{\tau}$.

TABLE VII

^{16}O Level	Neutron Exp[b]	Neutron TY	Proton Exp[a,b]	Proton TY
1s1		45.0	40±8	41.3
1p3	21.8	23.3	18.4	19.8
1p1	15.7	16.0	12.1	12.7
1d5	4.14	5.75	0.60	2.67
2s1	3.27	2.37	0.10	

^{40}Ca Level	Neutron Exp[b]	Neutron TY	Proton Exp[a,b]	Proton TY
1s1		61.4	50±11	53.7
1p3		42.5	34±6	35.0
1p1		37.6	34±6	30.2
1d5		24.6		17.6
2s1	18.1	18.5	10.9	11.5
1d3	15.6	16.5	8.3	9.61
1f7	8.36	8.78	1.4	2.22
2p3	6.2	3.69		
2p1		1.56		

^{48}Ca Level	Neutron Exp[b]	Neutron TY	Proton Exp[a,b]	Proton TY
1s1		63.5	55±9	59.7
1p3		44.8	35±7	42.4
1p1		41.2	35±7	38.4
1d5		27.0		25.0
2s1	12.55	20.2	15.3	17.6
1d3	12.52	19.4	15.7	17.5
1f7	9.94	10.7	9.6	8.84
2p3	5.14	5.14	1.9	2.00
2p1	3.11	2.89		
1f7		0.83		

(continued next page)

TABLE VII (continued)

^{208}Pb	Neutron		Proton	
Level	Exp.[b]	TY	Exp.[b]	TY
1s1		72.6		61.1
1p3		64.5		53.2
1p1		63.7		52.4
1d5		54.8		43.6
1d3		53.1		41.9
2s1		50.0		38.1
1f7		44.2		33.1
1f5		40.9		29.8
2p3		37.3		25.5
2p1		35.8		24.1
1g9		33.0	15.43	21.9
1g7		27.7	11.43	16.7
2d5		24.9	9.70	13.2
1h11		21.5	9.37	10.6
2d3		22.2	8.38	10.8
3s1		21.6	8.03	9.72
1h9	10.85	14.0	3.77	3.30
2f7	9.72	13.2	2.87	1.51
1i13	9.01	10.4	2.16	
3p3	8.27	9.51	0.95	
2f5	7.95	9.51	0.47	
3p1	7.38	8.14		
2g9	3.94	2.77		
1i11	3.15	0.79		
1j15	2.53			
3d5	2.36	0.33		
4s1	1.91	0.13		
2g7	1.45			
3d3	1.42			

(continued next page)

TABLE VII (continued)

^{90}Zr Level	Neutron Exp.[c]	Neutron TY	Proton Exp.[a]	Proton TY
1s1		71.3	54±8	60.9
1p3		57.0	43±8	47.9
1p1		55.1	43±8	45.6
1d5		41.9	27±8	33.7
1d3		37.5	27±8	29.0
2s1		35.7		26.8
1f7		27.0		19.3
1f5	13.5	19.5		11.8
1p3	13.1	19.7		11.0
2p1	12.6	17.1		8.66
1g9	12.0	12.9		5.38
2 5	7.2	6.13		
3s1	5.63	3.79		
2d3	4.88	2.93		
1g7	4.46	2.91		
1h11		2.16		

References:
a = (Jam+ 69)
b = (BM 69)
c = (Bas+ 68)

The experimental single-particle removal energies are compared with the eigenvalues ε_i calculated with interaction TY. Occupied levels appear above the dotted lines. The levels are denoted by $n\ell(2j)$.

TABLE VIII

Force	^{16}O 1p level splitting (MeV) Neutrons	Protons
TA	8.08	7.95
TB	6.61	6.52
TX	8.20	8.05
TY	7.30	7.16
TZ	6.59	6.48
Experiment	6.1	6.3

The 1p level splitting, $\varepsilon(1p\ 1/2) - \varepsilon(1p\ 3/2)$, of neutrons and protons in ^{16}O, for all five forces is compared with the difference in experimental (BM 69) single-particle removal energies.

LIST OF FIGURES

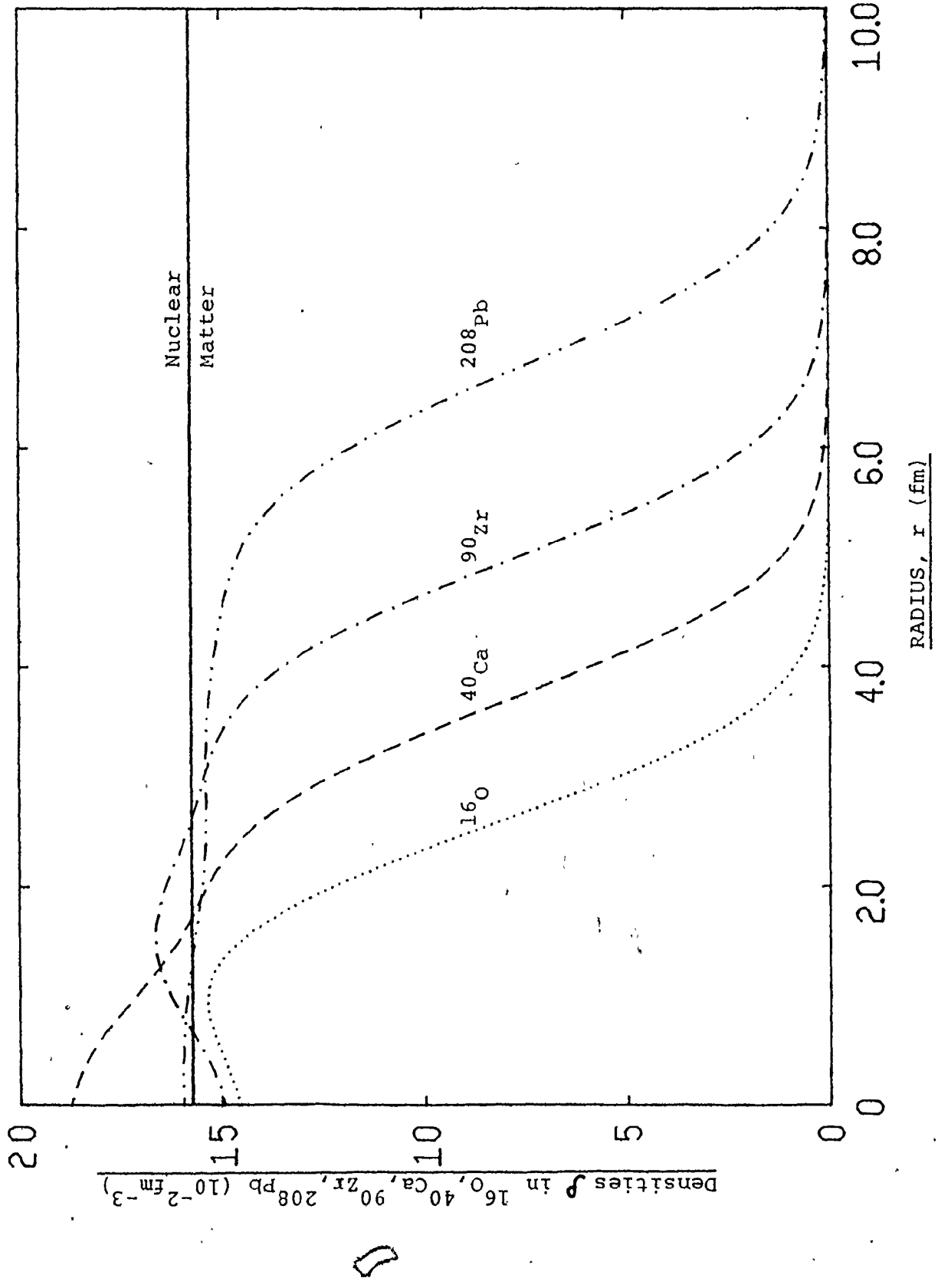
Densities ρ in 16O, 40Ca, 90Zr, 208Pb (10-2fm-3)
20
15
10
5
0
0
2.0
4.0
6.0
8.0
10.0
RADIUS, r (fm)
Nuclear
Matter
208Pb
90Zr
40Ca
16O

Figure 1

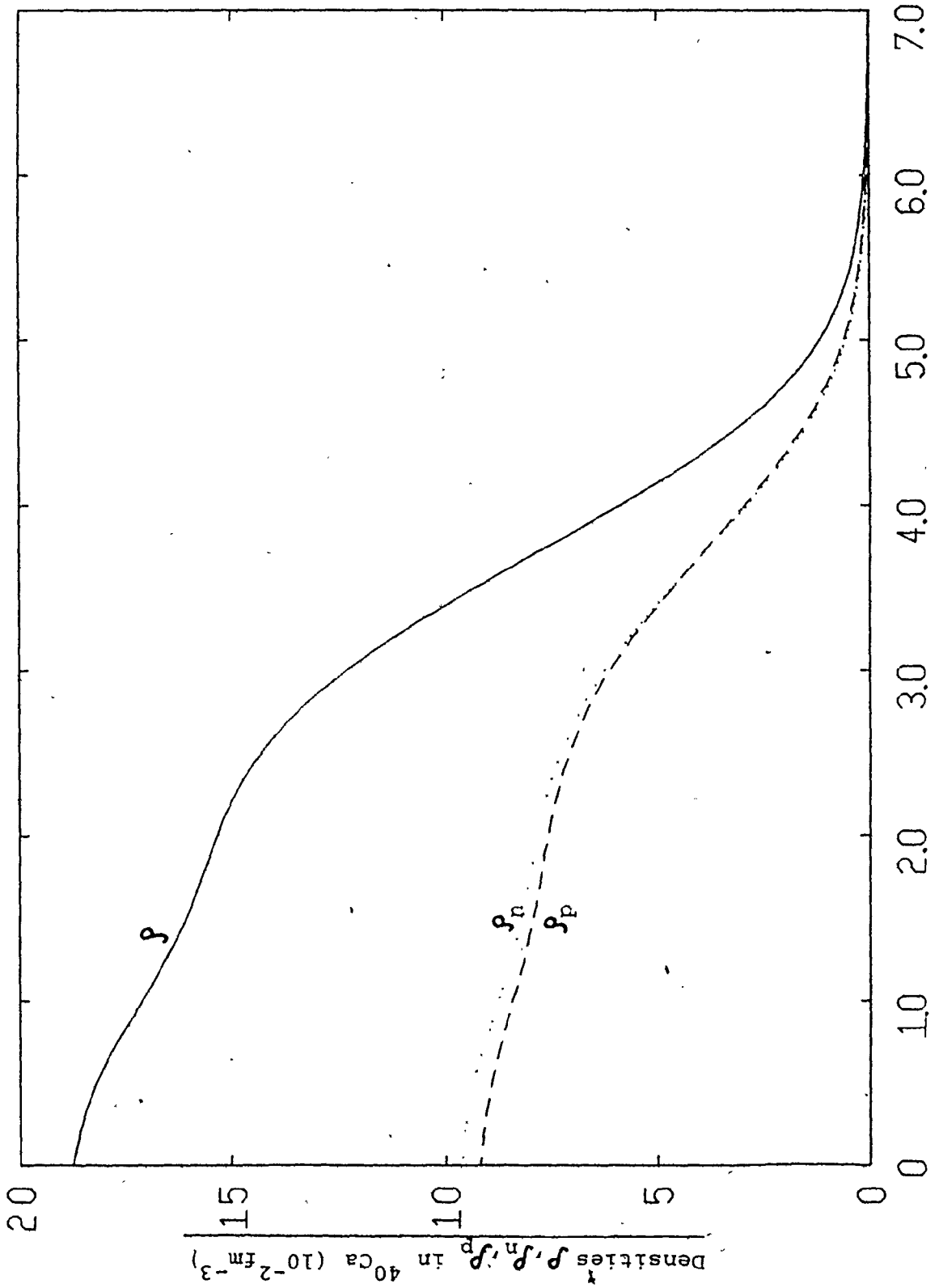
Densities ρ, ρn, ρp in 40Ca (10-2fm-3)
20
15
10
5
0
ρ
ρn
ρp
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
RADIUS, r (fm)

Figure 2

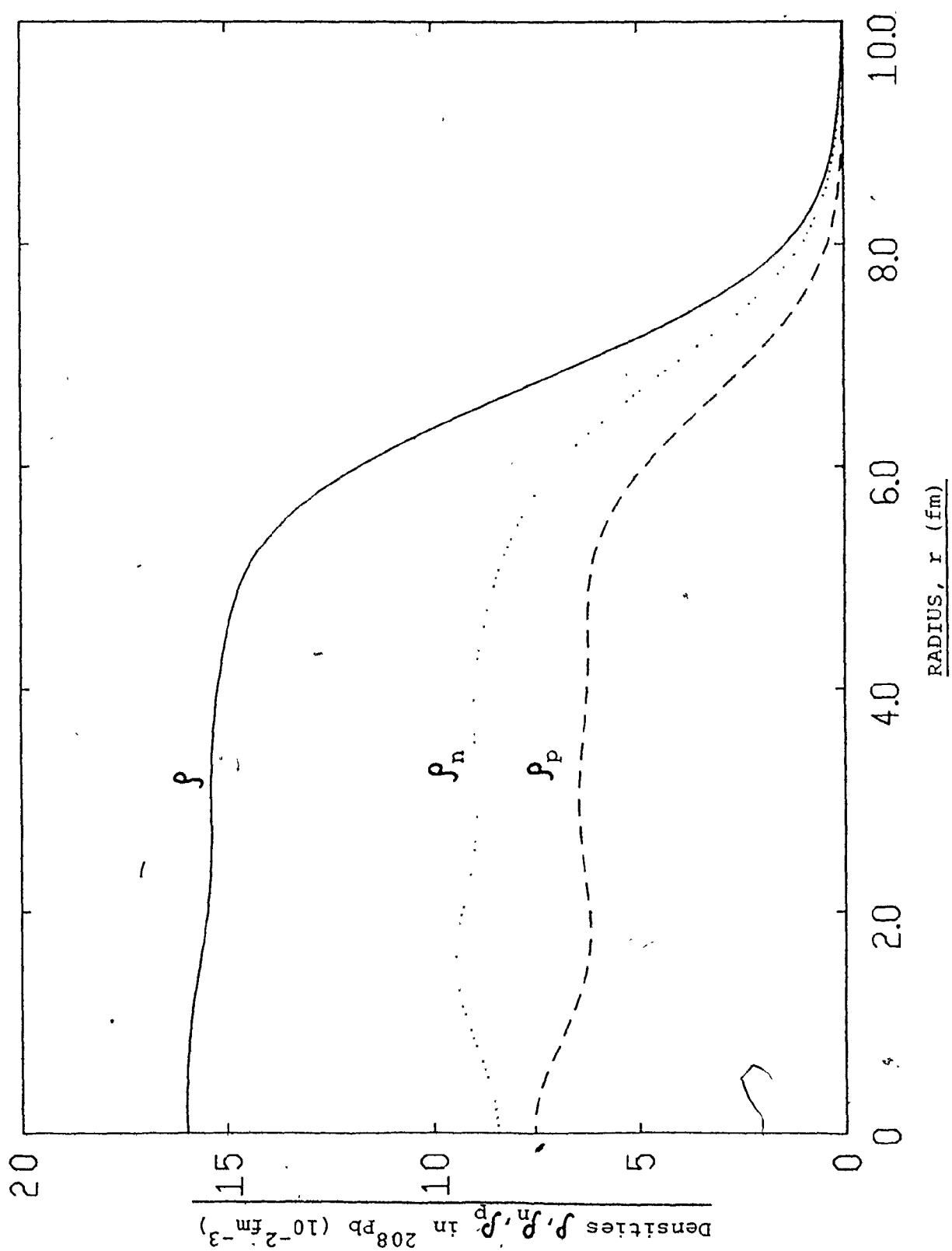
Densities ρ, ρn, ρp in 208Pb (10-2 fm-3)
RADIUS, r (fm)
ρ
ρn
ρp
0
5
10
15
20
2.0
4.0
6.0
8.0
10.0

Figure 3

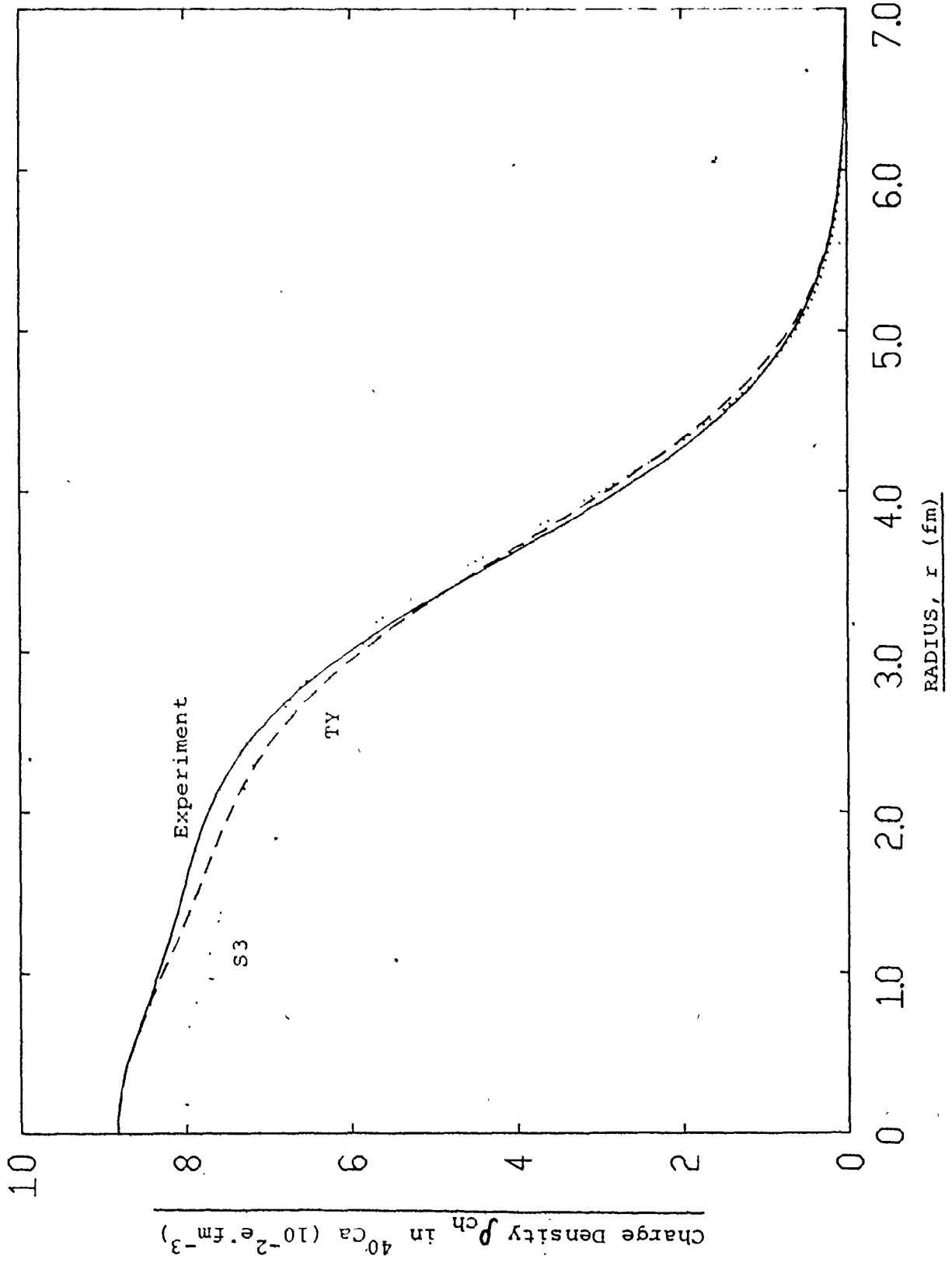
Charge Density ρ_{ch} in ^{40}Ca (10^{-2}e.fm^{-3})
10
8
6
4
2
0
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
RADIUS, r (fm)
Experiment
TY
S3

Figure 4

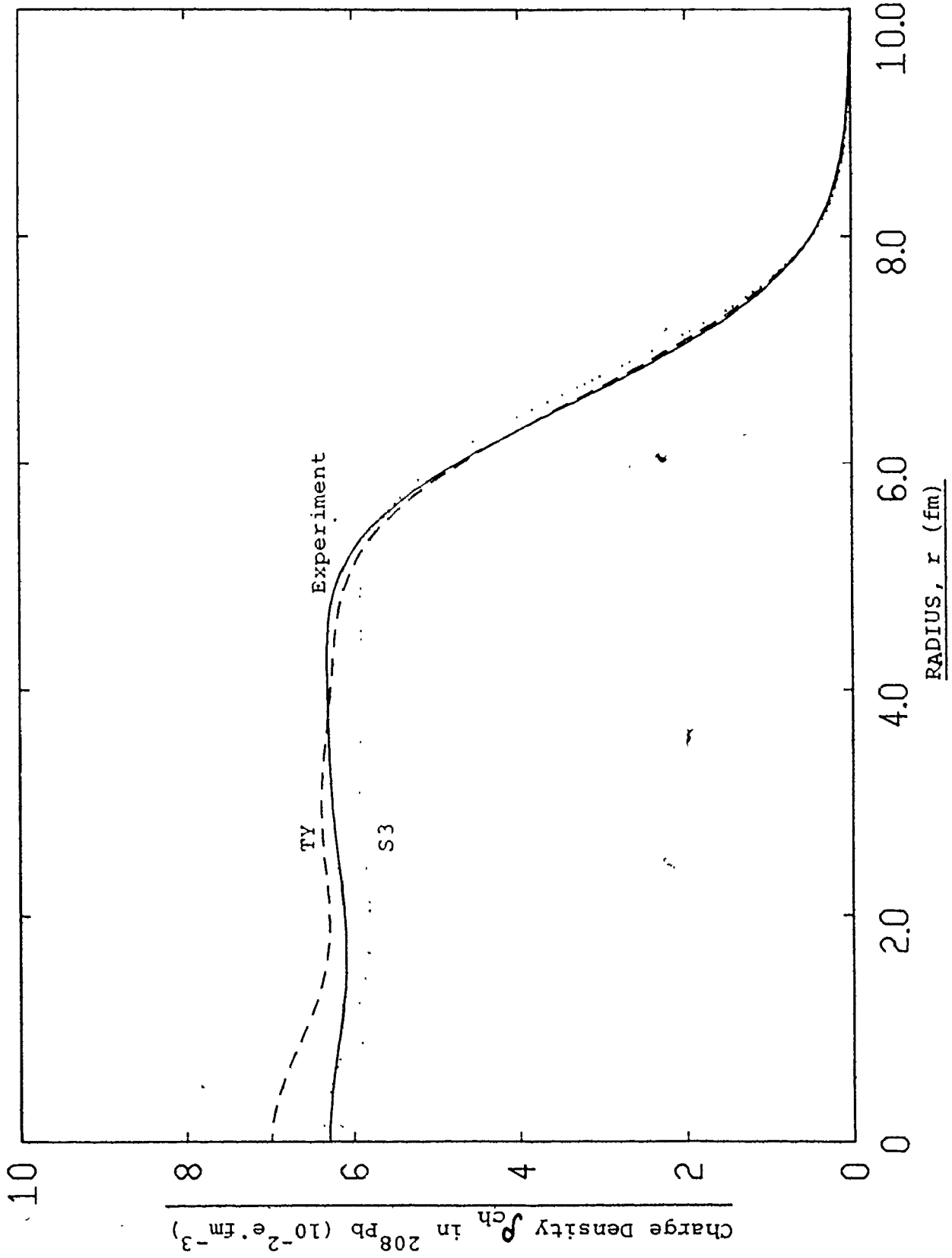
Charge Density ρ_{ch} in ^{208}Pb (10^{-2}e.fm^{-3})
RADIUS, r (fm)
Experiment
TY
S3
0
2.0
4.0
6.0
8.0
10.0
2
4
6
8
10

Figure 5

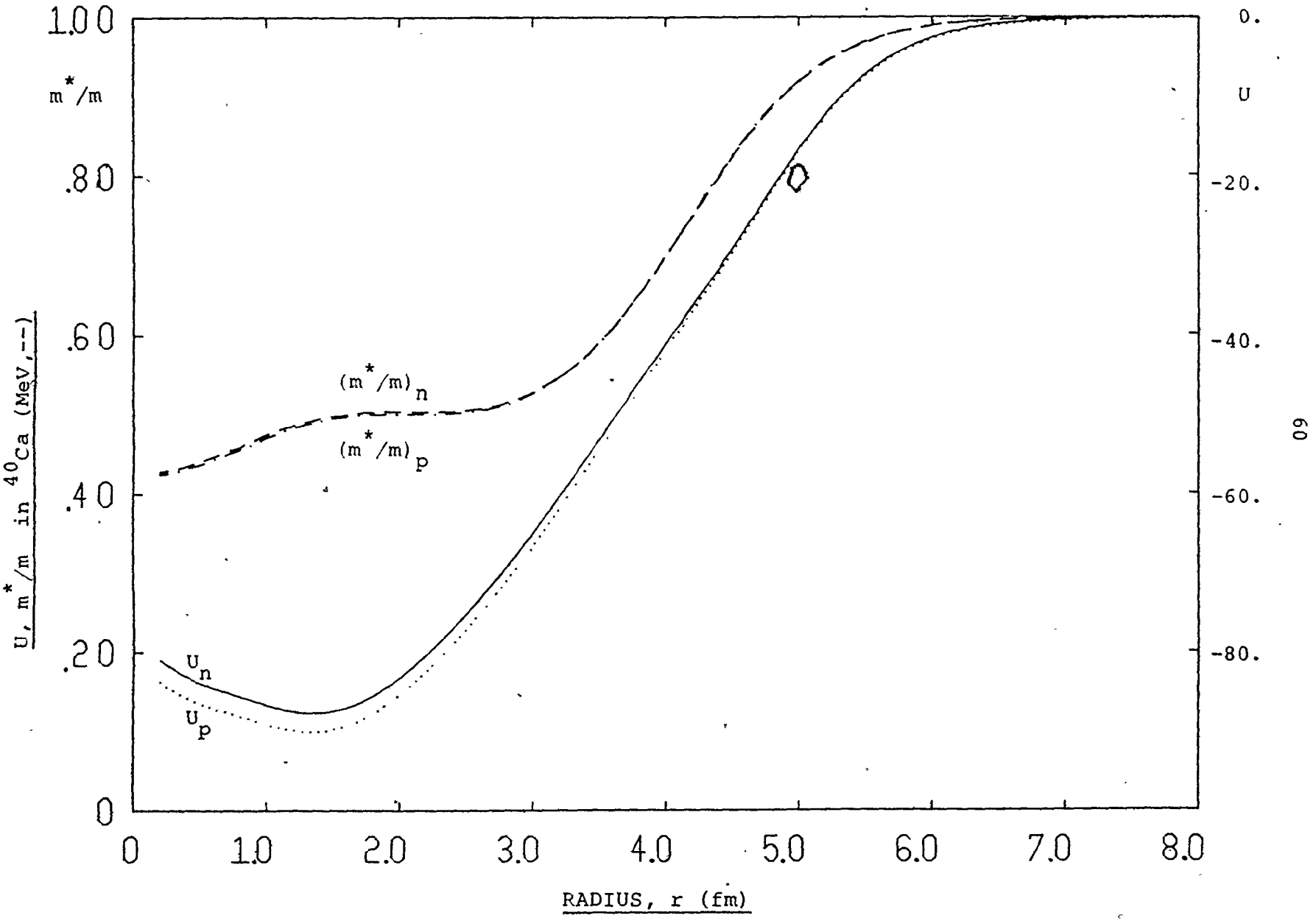
1.00
m*/m
.80
.60
.40
.20
0
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
RADIUS, r (fm)
U, m*/m in 40Ca (MeV,--)
0.
U
-20.
-40.
-60.
-80.
(m*/m)n
(m*/m)p
Un
Up

Figure 6

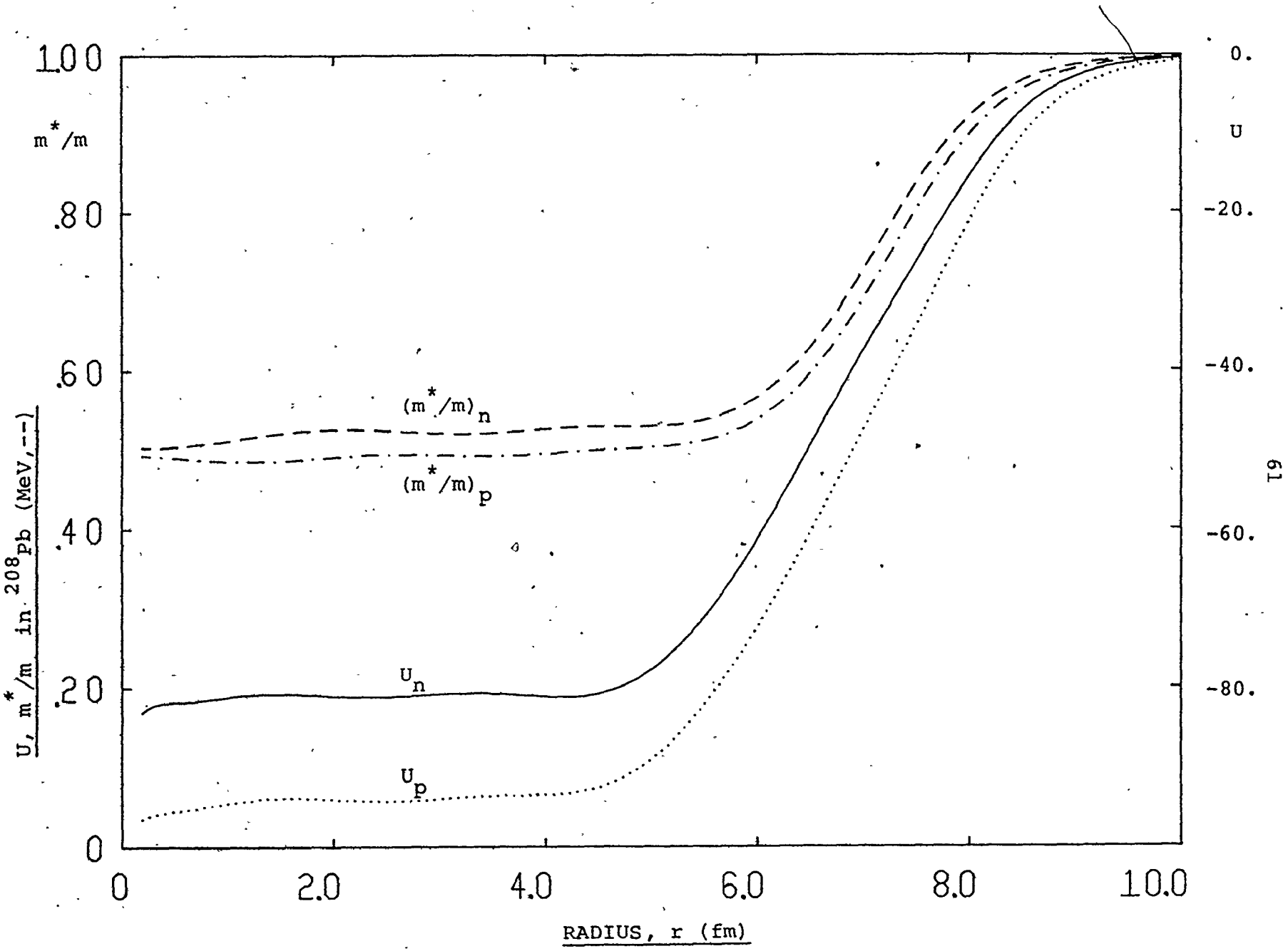
1.00
.80
.60
.40
.20
0
m*/m
0.
-20.
-40.
-60.
-80.
U
(m*/m)n
(m*/m)p
Un
Up
0
2.0
4.0
6.0
8.0
10.0
RADIUS, r (fm)
U, m*/m in 208Pb (MeV,--)

Figure 7

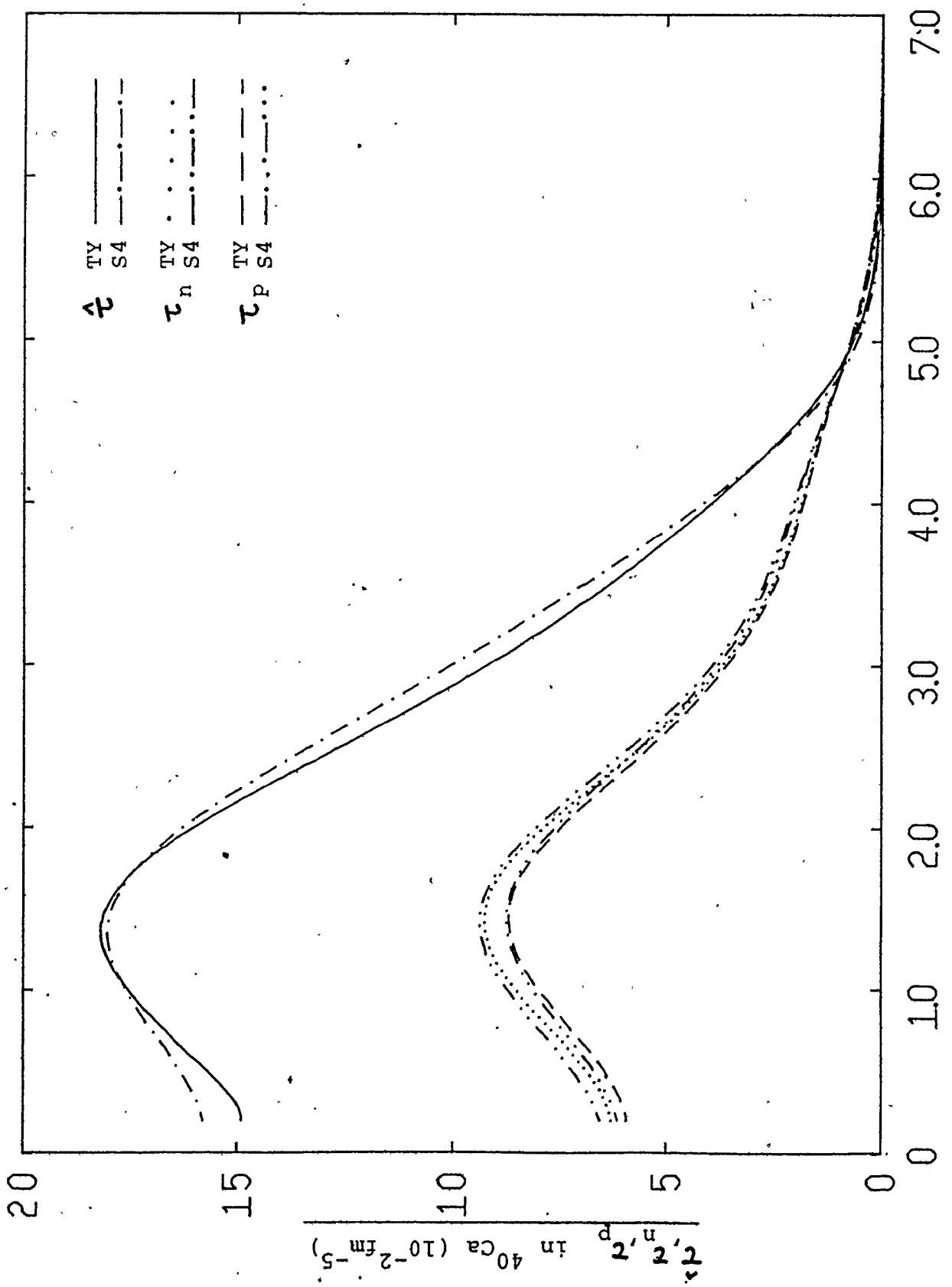
$\hat{\tau}$ TY
S4
τ_n TY
S4
τ_p TY
S4
$\hat{\tau}, \tau_n, \tau_p$ in ^{40}Ca (10^{-2}fm^{-5})
RADIUS, r (fm)
0
5
10
15
20
1.0
2.0
3.0
4.0
5.0
6.0
7.0

Figure 8

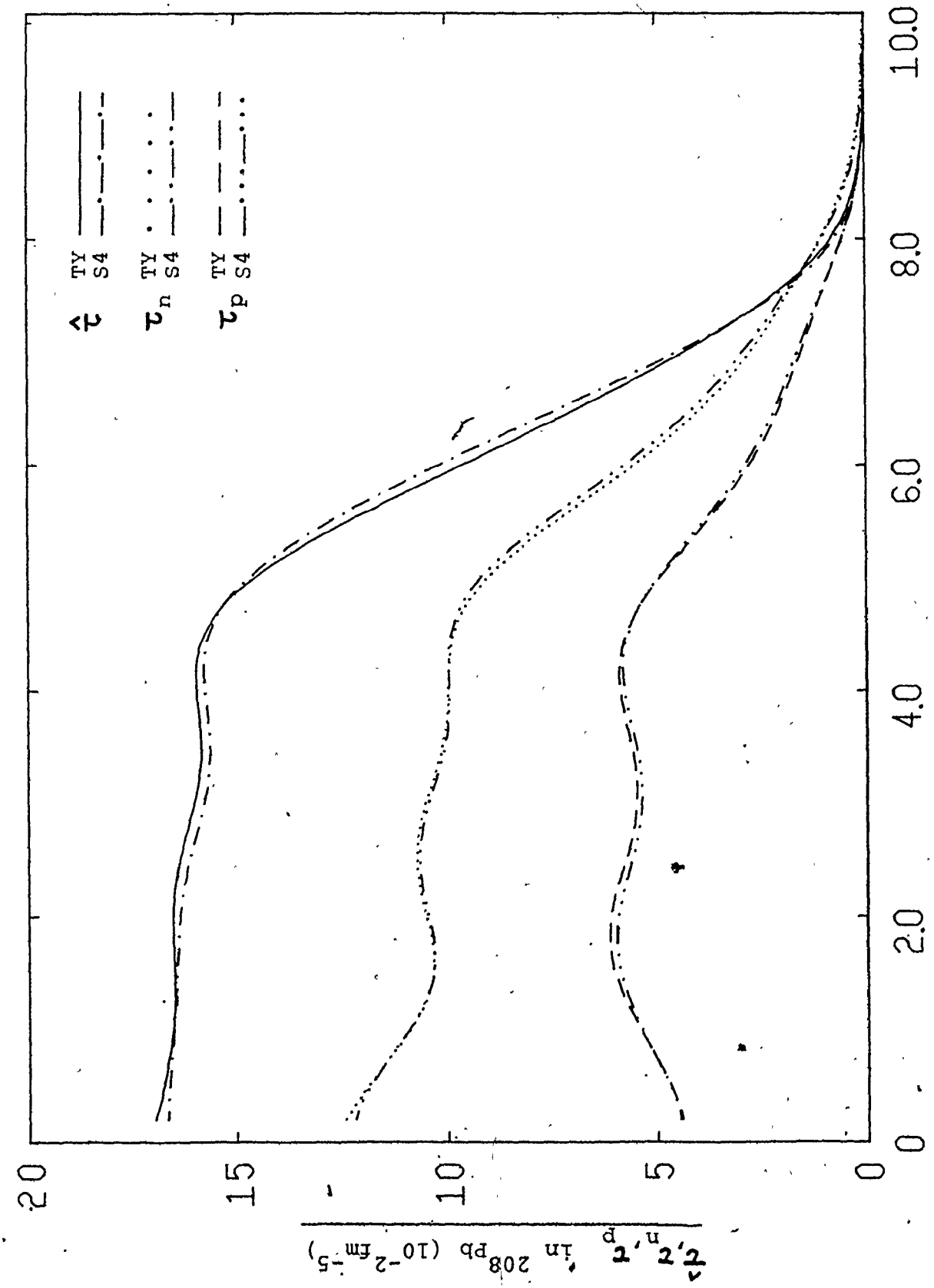
τ, τ_n, τ_p in ^{208}Pb (10^{-2} fm^{-5})
RADIUS, r (fm)
τ TY
τ S4
τ_n TY
τ_n S4
τ_p TY
τ_p S4
0
2.0
4.0
6.0
8.0
10.0
5
10
15
20

Figure 9

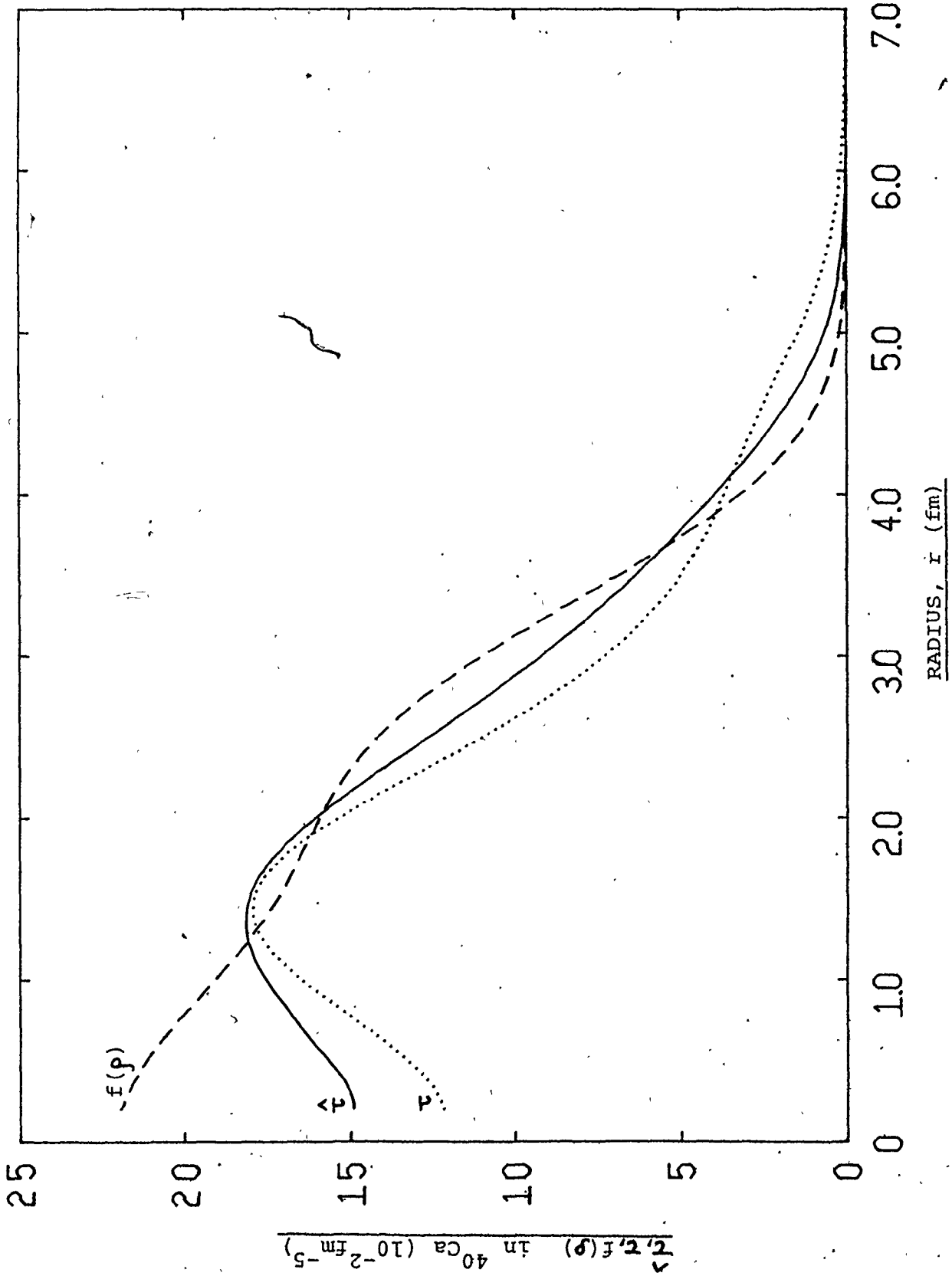

Figure 10

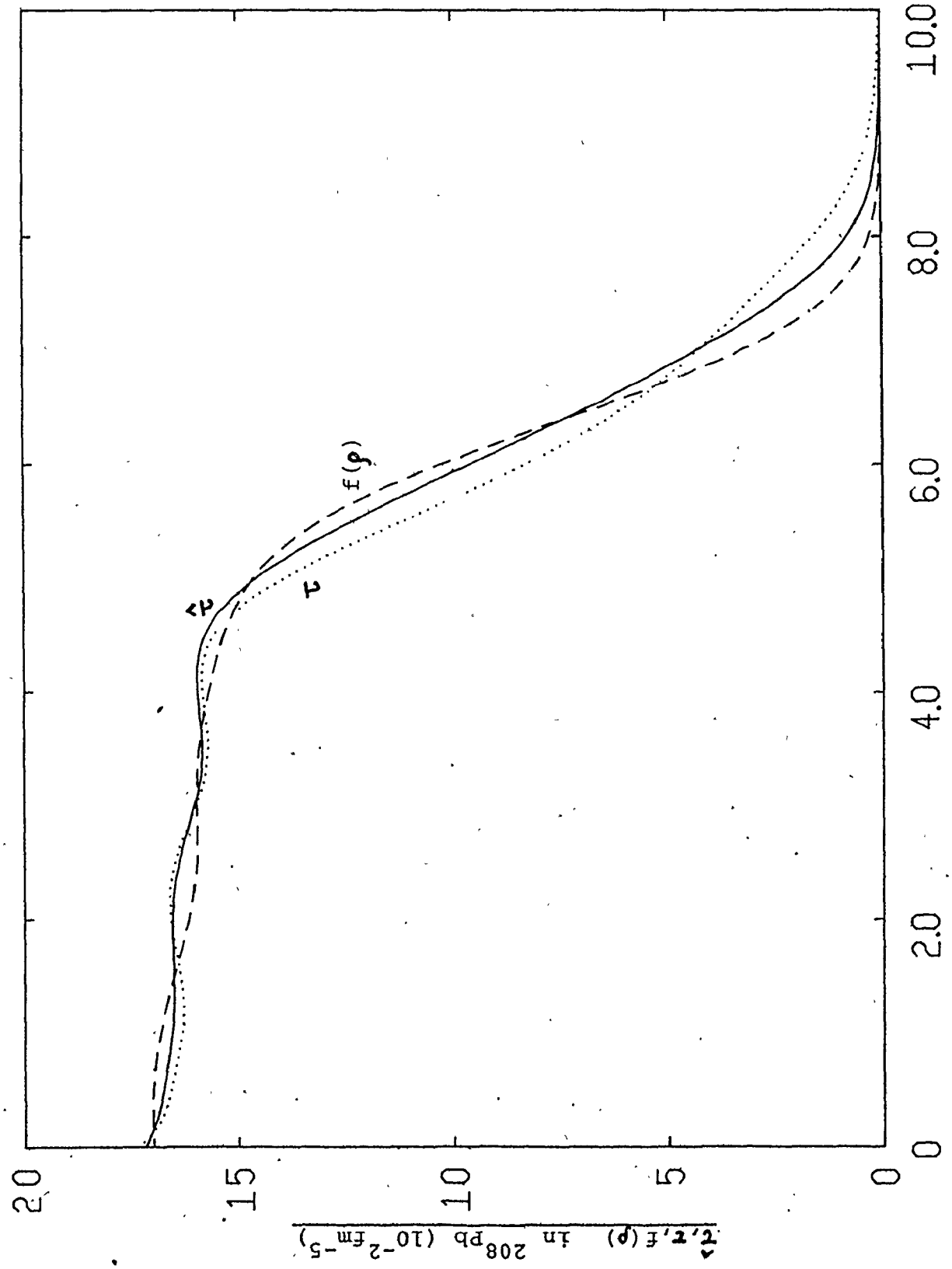

Figure 11

CHAPTER VII

CONCLUSIONS

In this work we have considered the Campy-Bouyssy Local Fermi Momentum $\hat{k}$ of eqn. (2.4) as an alternative prescription to the well-known Local Density Approximation, eqn. (2.2), for mapping the Fermi momentum dependence of the nuclear reaction matrix from the infinite to the finite system. This led to the concept of a $\hat{k}$-dependent effective nuclear interaction.

It was then shown that such a force would derive no rearrangement energy from its $\hat{k}$ dependence. One consequence of this fact is that, insofar as terms of order s^4 can be neglected in the standard Negele-Vautherin and the Campi-Bouyssy Density Matrix Expansions, either of these two approximations should give rise to no spurious rearrangement energy, when used in HF calculations, resulting from their potential energy density's dependence on ρ or $\hat{k}$, respectively.

However, since the rearrangement energy is an essential feature of a good effective interaction, one can say that in general the interaction should have dependence on ρ as well as on $\hat{k}$. This amounts to a dependence on quantities such as ρ, $\nabla^2\rho$, τ.

To show that a dependence on quantities other than ρ

is in fact feasible, an interaction which depends on $\hat{\tau} = .6\ \hat{k}^2\rho$ was developed, using the Skyrme force as a guide. Care must be exercised in choosing the numerical methods for solving the Hartree-Fock problem when using a force of this type. Nevertheless, a parameterization of this force, arbitrarily denoted TY, was developed, which gave results at least equal in quality to those of the various Skyrme forces, when used to calculate static nuclear properties in the HF approximation. It also possesses reasonable nuclear matter properties.

Thus, a dependence on quantities other than the density in the 'saturation term' of an effective nuclear interaction has been shown to be feasible.

APPENDIX A

In this appendix we present some equations relevant to the $\hat{\tau}^{\beta}$ dependent force chosen in chapter IV.

The phenomenological Hamiltonian to be used is written

$$\hat{H} = \sum_{i=1}^{A} \hat{t}_i + \sum_{i,j<i} (v_{ij} + v_{ij}^{(3)}) \ , \qquad (A.1)$$

where $t_i = -\frac{\hbar^2}{2m} \nabla_i^2$, and typically

$$v_{12} = t_0(1+x_0P_\sigma)\delta + \frac{1}{2} t_1(1+x_1P_\sigma)(k^{\dagger 2}\delta+\delta k^2) \qquad (A.2)$$

$$+ t_2(1+x_2P_\sigma)\underset{\sim}{k}^{\dagger}\cdot\delta\underset{\sim}{k} + iW(\underset{\sim}{\sigma}_1+\underset{\sim}{\sigma}_2)\cdot\underset{\sim}{k}^{\dagger}\times\delta\underset{\sim}{k}$$

$$+ e^2(q_1 + \tfrac{1}{2})(q_2 + \tfrac{1}{2})/(4\pi\epsilon_0 r_{12})$$

and

$$v_{12}^{(3)} = \frac{1}{6} t_3\hat{\tau}^{\beta}((\underset{\sim}{r}_1+\underset{\sim}{r}_2)/2)\delta(1+x_3P_\sigma) \ . \qquad (A.3)$$

Here $\underset{\sim}{k} = (\nabla_1-\nabla_2)/2i$, $P_\sigma = (1+\underset{\sim}{\sigma}_1\cdot\underset{\sim}{\sigma}_2)/2$, $\underset{\sim}{\sigma}$ is Pauli's spin matrix, $\delta = \delta(\underset{\sim}{r}_{12})$ and $\hat{\tau} \equiv \tau - \frac{1}{4}\nabla^2\rho$. The terms proportional to t_0, t_1, t_2, W become the Skyrme force with $t_3 = 0$ in the case $x_1 = x_2 = 0$. The motivation for $V_{12}^{(3)}$ is given in chapter IV.

The energy density $H(\underset{\sim}{r})$, which must satisfy $\int H(\underset{\sim}{r})d^3r = E_{TOT}$, is given in the HF approximation by:

$$H(\underset{\sim}{r}) = \frac{\hbar^2}{2m}\tau(\underset{\sim}{r}) + \sum_{i=0}^{3} H_i(\underset{\sim}{r}) + H_{LS}(\underset{\sim}{r}) + H_C(\underset{\sim}{r}) \qquad (A.4)$$

where the subscript i indicates proportionality to $t_0,\cdots,\bar{t}_3$. H_{LS} and $H_C = H_{CD} + H_{CEX}$ denote the spin-orbit and Coulomb energy densities. The contributions H_0, H_1, H_2, H_{LS}, H_C are all derived in (VB 72), except in that they have included neither x_1 nor x_2. The calculation of H_3 is exactly analogous to that of H_0, as is the derivation of (3.8) from (3.7). (Compare (A.3) with first term of (A.2) and H_0 with H_3 below.)

Listing all the contributions to H explicitly

$$\begin{aligned}
H_0 &= \tfrac{1}{2}\, t_0((1 + \tfrac{1}{2}\, x_0)\rho^2 - (\tfrac{1}{2} + x_0)(\rho_n^2 + \rho_p^2)) \\
H_1 &= \tfrac{1}{8}\, t_1((2\rho\tau - \tfrac{3}{2}\,\rho\nabla^2\rho)(1 + \tfrac{1}{2}\, x_1) + \\
&\quad + (\tfrac{3}{4}\,\rho_n\nabla^2\rho_n + \tfrac{3}{4}\,\rho_p\nabla^2\rho_p - \rho_n\tau_n - \rho_p\tau_p)(1+2x_1)) \\
H_2 &= \tfrac{1}{8}\, t_2((2\rho\tau + \tfrac{1}{2}\,\rho\nabla^2\rho)(1 + \tfrac{1}{2}\, x_2) + \\
&\quad + (\tfrac{1}{4}\,\rho_n\nabla^2\rho_n + \tfrac{1}{4}\,\rho_p\nabla^2\rho_p + \rho_n\tau_n + \rho_p\tau_p)(1+2x_2)) \qquad (A.5) \\
H_3 &= \tfrac{1}{12}\,\bar{t}_3\hat{\tau}^{\beta}((1 + \tfrac{1}{2}\, x_3)\rho^2 - (\tfrac{1}{2} + x_3)(\rho_n^2+\rho_p^2)) \\
H_{LS} &= -\tfrac{1}{2}\, W(\rho\nabla\cdot\underset{\sim}{J} + \rho_n\nabla\cdot\underset{\sim}{J}_n + \rho_p\nabla\cdot\underset{\sim}{J}_p) \\
H_{CD} &= \tfrac{1}{2}\,\rho_p V_c \equiv \tfrac{1}{2}\,\rho_p(\underset{\sim}{r}) \int \rho_p(\underset{\sim}{r}')e^2/(4\pi\varepsilon_0|\underset{\sim}{r}-\underset{\sim}{r}'|)d^3r' \\
H_{CEX} &= -\tfrac{3}{4}\,(3/\pi)^{1/3}e^2\rho_p^{4/3}/(4\pi\varepsilon_0)\ .
\end{aligned}$$

In the Coulomb exchange term the Slater approximation has been used. Following (VB 72) a small spin-orbit contribution arising from the terms of (A.2) proportional to t_1 and t_2 has been neglected.

Varying the single-particle functions ϕ_i, subject to the constraint of normalization, so that E_{TOT} is minimized, produces the HF equations

$$-\nabla\cdot\left(\frac{\hbar^2}{2m_q^*}\nabla\phi_i\right) + (U_q - iW_q\cdot\nabla\times\sigma)\phi_i = \varepsilon_i\phi_i \ , \qquad (A.6)$$

in which the effective mass, potential, and spin-orbit form factor are all position dependent and are given respectively by

$$\begin{aligned}
\frac{\hbar^2}{2m_q^*} &= \frac{\hbar^2}{2m} + \frac{1}{4}\left(t_1\left(1+\frac{1}{2}x_1\right) + t_2\left(1+\frac{1}{2}x_2\right)\right)\rho \\
&\quad + \frac{1}{8}\left(t_2(1+2x_2) - t_1(1+2x_1)\right)\rho_q + \partial H_3/\partial\hat{\tau} \ , \\
U_q &= t_0\left(\left(1+\frac{1}{2}x_0\right)\rho - \left(x_0+\frac{1}{2}\right)\rho_q\right) + \frac{1}{4}\left(t_1\left(1+\frac{1}{2}x_1\right) + t_2\left(1+\frac{1}{2}x_2\right)\right)\tau \\
&\quad + \frac{1}{8}\left(t_2(1+2x_2) - t_1(1+2x_1)\right)\tau_q - \frac{1}{8}\left(3t_1\left(1+\frac{1}{2}x_1\right) - t_2\left(1+\frac{1}{2}x_2\right)\right)\nabla^2\rho \\
&\quad + \frac{1}{16}\left(3t_1(1+2x_1) + t_2(1+2x_2)\right)\nabla^2\rho_q - \frac{1}{2}W(\nabla\cdot J + \nabla\cdot J_q) \\
&\quad + \left(q+\frac{1}{2}\right)\left(V_c - e^2(3\rho_p/\pi)^{1/3}/4\pi\varepsilon_0\right) + \frac{\partial H_3}{\partial\rho_q} - \frac{1}{4}\nabla^2\frac{\partial H_3}{\partial\hat{\tau}} \ , \qquad (A.7) \\
W_q &= \frac{1}{2}W(\nabla\rho + \nabla\rho_q) \ .
\end{aligned}$$

Here q denotes p(n) or $\frac{1}{2}$ $(-\frac{1}{2})$ according to the charge index q_i of the single particle state i. All the terms in (A.7) except

those proportional to $\bar{t}_3$ are either derived in (VB 72) or are straightforward extensions thereof.

We now derive the contributions to (A-7) arizing from $H_3 \equiv \hat{\tau}^{\beta}(\tau, \nabla^2\rho) \cdot \chi(\rho_n, \rho_p)$. In the variation one performs to this term of H

$$\frac{\partial H_3}{\partial \phi_i^*} - \nabla \cdot \frac{\partial H_3}{\partial \nabla \phi_i^*} + \nabla^2 \frac{\partial H_3}{\partial \nabla^2 \phi_i^*} \cdot$$

Recalling the expression (3.10) for $\hat{\tau}$, we evaluate

$$\frac{\partial H_3}{\partial \phi_i^*} = \frac{\partial H_3}{\partial \rho_i} \frac{\partial \rho_i}{\partial \phi_i^*} + \frac{\partial H_3}{\partial \hat{\tau}} \frac{\partial \hat{\tau}}{\partial \phi_i^*} = \frac{\partial H_3}{\partial \rho_i} \phi_i - \frac{1}{4} \frac{\partial H_3}{\partial \hat{\tau}} \nabla^2 \phi_i \quad ,$$

$$\nabla^2 \frac{\partial H_3}{\partial \nabla^2 \phi_i^*} = \nabla^2 \left(\frac{\partial H_3}{\partial \hat{\tau}} \frac{\partial \hat{\tau}}{\partial \nabla^2 \phi_i^*}\right) = - \frac{1}{4} \nabla^2 \left(\frac{\partial H_3}{\partial \hat{\tau}} \phi_i\right) \quad ,$$

$$- \nabla \cdot \frac{\partial H_3}{\partial \nabla \phi_i^*} = - \nabla \cdot \left(\frac{\partial H_3}{\partial \hat{\tau}} \frac{1}{2} \nabla \phi_i\right) \quad . \qquad \text{(A.8)}$$

From the first term, we see that $\partial H_3/\partial \rho_i$ goes into the potential U_q as stated in (A.7). Adding the next two contributions (with $X \equiv \partial H_3/\partial \hat{\tau}$):

$$- \frac{1}{4} \left(X \nabla^2 \phi_i + \nabla^2 (X \phi_i)\right)$$

$$= - \frac{1}{4} \left(X \nabla^2 \phi_i + \nabla \cdot (X \nabla \phi_i) + (\nabla^2 X) \phi_i + \nabla X \cdot \nabla \phi_i\right)$$

$$= - \frac{1}{4} \left((\nabla^2 X) \phi_i + 2 \nabla \cdot (X \nabla \phi_i)\right) \quad .$$

The first of these terms completes the potential U_q, and the

last term, when combined with the idential (A.8), is $-\nabla\cdot(X\nabla\phi_i)$. This then produces the contribution of $\partial H_3/\partial\hat{\tau}$ to $\hbar^2/2m_q^*$ in (A.7).

For spherical nuclei, one then makes the ansatz ($i \equiv \alpha;m \equiv n,\ell,j,q;m$)

$$\phi_{\alpha;m} = r^{-1}\, u_\alpha(r)\mathcal{Y}_{\ell,j,m}(\Omega,\sigma)\chi_q(\tau)$$

in (A.6). As in (VB 72), the radial wavefunctions u_α then must satisfy the following second order differential equations:

$$\frac{\hbar^2}{2m_q^*}\left[-u'' + \frac{\ell(\ell+1)}{r^2}u\right] - \left(\frac{\hbar^2}{2m_q^*}\right)' u' + \left[U_q + \frac{1}{r}\left(\frac{\hbar^2}{2m_q^*}\right)' + \right.$$

$$\left. + \left(j(j+1) - \ell(\ell+1) - \frac{3}{4}\right)W_q/r\right]u = \varepsilon u \ .$$

The self-consistent solution can then be found by using an iterative DME-HF computer programme.

APPENDIX B

In this appendix, we derive the contribution of the parameters x_1, x_2, $\bar{t}_3$ to the NM symmetry energy co-efficient ε_1, which was defined in chapter V by

$$\varepsilon_1 = \lim_{\alpha \to 0} \frac{E_{NM}(\alpha) - E_{NM}(0)}{\alpha^2} \qquad (B.1)$$

Recall that $E_{NM} = H_{NM}/\rho$ and $\alpha \equiv (\rho_n - \rho_p)/\rho$, so that $\rho_{n/p} = (\rho/2)(1 \pm \alpha)$.

It will be necessary to find τ_q $(q = n,p)$ in terms of α. Recalling (5.1) and (5.2), consider

$$\tau_n = \frac{3}{5} k_{Fn}^3 \rho_n = \frac{3}{5} (3\pi^2)^{2/3} \rho_n^{5/3} ,$$

and

$$\rho_n^{5/3} = (\rho/2)^{5/3}(1+\alpha)^{5/3}$$

$$= (\rho/2)^{5/3}(1 + \frac{5}{3}\alpha + \frac{5}{9}\alpha^2 + O(\alpha^3)) .$$

Thus

$$\tau_n = \frac{3}{10} (3\pi^2/2)^{2/3} \rho^{5/3}(1 + \frac{5}{3}\alpha + \frac{5}{9}\alpha^2 + O(\alpha^3)) .$$

Similarly by replacing α with $-\alpha$ one finds

$$\tau_p = \frac{3}{10} (3\pi^2/2)^{2/3} \rho^{5/3}(1 - \frac{5}{3}\alpha + \frac{5}{9}\alpha^2 + O(\alpha^3))$$

so that

$$\tau = \frac{3}{5}(3\pi^2/2)^{2/3}\rho^{5/3}(1 + \frac{5}{9}\alpha^2 + O(\alpha^3)) \quad . \qquad (B.2)$$

(i) Contribution due to x_1: From (A-5) we see that the contribution to E_{NM} due to x_1 is

$$E_{x1,NM} = H_{x1,NM}/\rho = \frac{1}{8}x_1t_1(\tau - 2(\rho_n\tau_n+\rho_p\tau_p)/\rho) \quad ,$$

which vanishes in the event $\rho_n = \rho_p$, i.e. $E_{x1,NM}(0) = 0$. Generally

$$E_{x1,NM}(\alpha) = \frac{1}{8}x_1t_1\frac{3}{10}(\frac{3\pi^2}{2})^{2/3}\rho^{5/3}[2 + \frac{10}{9}\alpha^2 -$$

$$- (1+\frac{5}{3}\alpha + \frac{5}{9}\alpha^2)(1+\alpha) - (1-\frac{5}{3}\alpha + \frac{5}{9}\alpha^2)(1-\alpha)]$$

$$= \frac{1}{8}x_1t_1\frac{3}{10}(\frac{3\pi^2}{2}\rho)^{2/3}\rho(-10/3)\alpha^2$$

$$= -\frac{1}{8}x_1t_1k_F^2\rho\alpha^2 \quad .$$

Hence, by (B-1), the contribution of this term to ε_1 is

$$-\frac{1}{8}x_1t_1k_F^2\rho \quad . \qquad (B-3)$$

(ii) Contribution due to x_2: Again from (A-5) we see that

$$E_{x2,NM} = \frac{1}{8}t_2x_2(\tau + 2(\rho_n\tau_n+\rho_p\tau_p)/\rho)$$

which equals $\frac{1}{4}t_2x_2\tau$ when $\alpha = 0$. Otherwise

$$E_{x2,NM}(\alpha) = \frac{1}{8}\, t_2x_2\, \frac{3}{10}\, (\frac{3\pi^2}{2})^{2/3} \rho^{5/3} (2 + \frac{10}{9}\, \alpha^2 + (2 + \frac{10}{9}\, \alpha^2 + \frac{10}{3}\, \alpha^2))$$

$$= \frac{1}{8}\, t_2x_2\, \frac{3}{10}\, (\frac{3\pi^2}{2}\, \rho)^{2/3} \rho (4 + \frac{50}{9}\, \alpha^2)$$

$$= \frac{1}{16}\, t_2x_2\tau (4 + \frac{50}{9}\, \alpha^2)$$

Hence, by (B-1) the contribution to ε_1 is

$$\frac{5}{24}\, t_2x_2\, \rho\, k_F^2 \,. \qquad \text{(B-4)}$$

(iii) Contribution due to $\bar{t}_3$: From (A-5) one has

$$E_{\bar{t}3,NM} = \frac{1}{12}\, \bar{t}_3\tau^\beta \{1 + \frac{1}{2}\, x_3)\rho - (\frac{1}{2} + x_3)(\rho_n^2 + \rho_p^2)/\rho\} \qquad \text{(B-5)}$$

which equals $\frac{1}{16}\, \bar{t}_3\tau^\beta\rho$ when $\alpha = 0$. Generally we have from (B-2) that

$$\tau^\beta = (2k_F^5/5\pi^2)^\beta (1 + \frac{5}{9}\, \alpha^2)^\beta$$

$$= (2k_F^5/5\pi^2)^\beta (1 + \frac{5}{9}\, \beta\alpha^2 + O(\alpha^4))$$

and the part of (B-5) in curly parentheses equals

$$\rho(1 + \frac{1}{2}\, x_3 - (\frac{1}{2} + x_3)\frac{1}{4}((1+\alpha)^2 + (1-\alpha)^2)$$

$$= \rho(\frac{3}{4} - \frac{1}{2}\, (\frac{1}{2} + x_3)\alpha^2) \,.$$

Substituting these into (B-5) yields

$$E_{\bar{t}3,NM}(\alpha) = \frac{1}{24}\, \bar{t}_3\rho(2k_F^5/5\pi^2)^\beta (1 + \frac{5}{9}\, \beta\alpha^2)(\frac{3}{2} - (\frac{1}{2} + x_3)\alpha^2) \,.$$

Hence, by (B-1) the contribution to ε_1 is

$$\frac{1}{24}\,\bar{t}\,\rho\,\tau^{\beta}\,\left(\frac{5}{6}\,\beta - x_3 - \frac{1}{2}\right) . \qquad \text{(B-6)}$$

The terms in (B-3), (B-4), and (B-6) are just the desired new contributions appearing in equation (5.12).

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