THE HARMONIC OSCILLATOR APPROXIMATION
TO THE DENSITY MATRIX

By

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ABSTRACT

We derive an approximate form for the angle averaged single particle density matrix for particles in a central potential. It is a Taylor series expansion in the interparticle distance $|\underset{\sim}{S}|$ based on the exact density matrix for particles in a harmonic oscillator potential. This form is also shown to be exact for particles in a linear and quadratic potential in one dimension.

We show the relation between this approximation and previous ones derived by Negele and Vautherin, Campi and Bouyssy, and Jennings. All these approximations agree with the exact angle averaged density matrix up to the S^2 coefficient of their respective Taylor series expansion in $|\underset{\sim}{S}|$. We compare the coefficients of S^4 and higher powers of S within each approximation to show the connections between them.

We then check, numerically, the S^4 coefficients of the various approximations with the exact coefficient. In one dimension we use the Eckart potential and in three dimensions we use the Woods Saxon. All three give reasonably good approximations to the exact S^4 coefficient, with the exception of the Negele Vautherin form in one dimension.

Suggestions for putting the harmonic oscillator approximation into a form amenable to calculating exchange integrals are made.

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INTRODUCTION

The nucleus is a strong interacting many body system. Therefore it is not clear that nucleons can be described as independent noninteracting particles in a central potential well. However, the success of the shell model indicates that it is a good approximation to think of the nucleus in terms of independent particles. In this case we would like to find the "best" single particle orbitals for the nucleons. The single particle orbitals could be obtained from a phenomenological one-body potential like the harmonic oscillator or the Woods-Saxon potential. A more satisfactory approach would be to start from the two-nucleon interaction that fits the scattering data, and construct an effective (G-matrix type) interaction with which one could perform a Hartree-Fock calculation to obtain the self-consistent one-body field. Such one-body potentials are density-dependent in character.

The Hartree Fock theory involves the calculation of exchange matrix elements. For a central two body interaction he exchange matrix element may be written as:

$$\langle E\rangle_{EX} = - \iint \overline{\rho^2(\underset{\sim}{Q},\underset{\sim}{S})}\, v(S)\, d^3Q\, d^3S \qquad (1)$$

where v(S) is the 2 body central potential, $\rho(\underset{\sim}{Q},\underset{\sim}{S})$ is defined in (1.2), and the angle average is defined in appendix B.

Writing the exchange matrix element in the form of equation (1) represents a simplification over a full Hartree Fock treatment since we may do the $\underset{\sim}{S}$ integration rather easily, and hence be left with a "local" exchange term. This local term reduces the work done in a variational calculation by a large amount.

This provides the motivation for the present work. Some approximations to $\overline{\rho^2(\underset{\sim}{Q},\underset{\sim}{S})}$ must be proposed in order that we may actually do the calculation in (1). This is rather difficult. However, it can be shown that $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}^2$ is identical to $\overline{\rho^2(\underset{\sim}{Q},\underset{\sim}{S})}$ when expanded in a Taylor series of the interparticle distance $\underset{\sim}{S}$ up to S^2. Hence we make an approximation on $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}$ and square it, with errors due to squaring appearing in S^4 and higher coefficients.

Several forms have been proposed for $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}$ which are appropriate for nuclear calculations. Negele and Vautherin (1972) derived a form (referred to as the NVA) based on a plane wave expansion. The NVA has been used in many calculations to date (Negele and Vautherin (1972,1975); Sprung et al (1975), Treiner and Krivine (1976)). Reasonable agreement was obtained for the gross properties of several nuclei. This leads us to believe that the approach is a useful one.

Campi and Bouyssy (1978), modified the Negele Vautherin form into a Slater-like form (referred to as the CBA). This has been checked in an analytically solvable model by Bhaduri and Sprung (1978). The CBA was found to give better exchange energy matrix elements for a fixed potential and was easier to use in comparison with the NVA. However, the CBA has a more complicated dependence on density than the NVA. Thus, to date, no one has reported a variational calculation using this form .

Jennings (1978) derived a semi-classical form for $\rho(\underset{\sim}{Q},\underset{\sim}{S})$ (with the explicit angular dependence on $\underset{\sim}{S}$ still present) based on the extended Thomas Fermi approximation. No reports have yet appeared using this in a calculation.

In the present work we consider a new form for the density matrix based on the exact density matrix for particles in a harmonic oscillator potential. The finite nucleus consists of particles in bound states which are known to be reasonably well approximated by harmonic oscillator wavefunctions. This was the rationale behind our approach.

In chapter one we derive the harmonic oscillator approximation (HOA) to the density matrix by direct analogy with the exact form for the density matrix of particles in a harmonic oscillator well. As the exact density matrix in this case is known only in a Taylor series in the interparticle distance $\underset{\sim}{S}$, the HOA is thus given as a Taylor series in both one and three dimensions. The exact density matrix for particles in a linear and a quadratic potential in one dimension are shown to have the same form as the HOA in appendix A. This led us to believe that the approximation ought to be reasonably good in the interior of the nucleus where the potential is reasonably "flat" due to saturation.

In chapter 2 we use a semiclassical approximation on the HOA to obtain it in a local form. This allowed us to compare the HOA to the other approximations mentioned above. The relationship between the approximations is checked term by term in a Taylor series expansion in S for each approximation.

In chapter 3 we calculate the density matrix in the HOA, the CBA, and the NVA for two model one body potentials in three dimensions and a one body potential in one dimension. These were compared with the exact angle averaged density matrix as given in appendix B in three dimensions and expression (1.15) in one dimension.

The one dimensional results show that the HOA and CBA are reasonably good, but the NVA is not. The three dimensional results show that the HOA is quite accurate, particularly in the interior. It confirms the findings of Campi and Bouyssy (1978A) that the CBA is more accurate in the tail. No calculation of matrix elements are given since in its present form, the HOA is not amenable to such calculation.

The final section of chapter 3 is devoted to a discussion of the results and suggestions of further work to be done in this area.

CHAPTER 1

THE HARMONIC OSCILLATOR APPROXIMATION TO THE DENSITY MATRIX

INTRODUCTION

In nuclear physics short range forces and correlations are important. Hence, it is useful to know the expansion of the density matrix $\rho(\underset{\sim}{R},\underset{\sim}{R}')$ in the relative coordinate $\underset{\sim}{S} = \underset{\sim}{R}-\underset{\sim}{R}'$. Even when this expansion does not converge rapidly to the density matrix $\rho(\underset{\sim}{R},\underset{\sim}{R}')$, it is still of use in calculating matrix elements of short range interactions, such as those which are found in nuclei.

In this chapter we define the single particle density matrix, $\rho(\underset{\sim}{R},\underset{\sim}{R}')$ for the ground-state of a many-fermion system in the independent-particle model and calculate it explicitly for the harmonic oscillator potential. An expression of the exact harmonic oscillator density matrix in the relative coordinate $\underset{\sim}{S}$ is then obtained, and the coefficients are rewritten in terms of the kinetic energy density $\tau(\underset{\sim}{R})$ and gradients of the density. We then propose to write the expansion of the density matrix for a general potential in an analogous form. We chose the harmonic oscillator potential as a guide for the simplicity of the result obtained, and also because it is known that harmonic oscillator wavefunctions are a good approximation to the true nuclear wave function in many cases (de Shalit and Feshbach, 1974).

i) Definitions

We begin with the single particle density matrix in the spatial representation. Formally it is defined as

$$\rho(\underset{\sim}{R}_1,\underset{\sim}{R}_1') = \int \Psi_0^*(\underset{\sim}{R}_1,\ldots,\underset{\sim}{R}_N)\Psi_0(\underset{\sim}{R}_1',\ldots,\underset{\sim}{R}_N)\,d^3R_2\ldots d^3R_N$$

(Landau and Lifshitz, 1977). However, within the independent particle approximation $\Psi_0(\underset{\sim}{R}_1,\ldots,\underset{\sim}{R}_N)$ is a Slater determinant and therefore the density matrix reduces to:

$$\rho(\underset{\sim}{R},\underset{\sim}{R}') = \sum_{i=0}^{N} g_i\psi_i(\underset{\sim}{R})\psi_i^*(\underset{\sim}{R}') \tag{1}$$

where the ψ_i are eigenfunctions of a single particle Hamiltonian, $\psi_N(r)$ is the eigenstate with the greatest energy which is occupied, and g_i is the occupation number of the i'th orbital. In terms of the centre of mass (COM) and relative coordinates, we have

$$\rho(\underset{\sim}{Q},\underset{\sim}{S}) = \sum_{i=0}^{N} g_i\psi_i(\underset{\sim}{Q} + \frac{\underset{\sim}{S}}{2})\psi_i^*(\underset{\sim}{Q} - \frac{\underset{\sim}{S}}{2}) \tag{2}$$

with $\underset{\sim}{Q} = (\underset{\sim}{R}+\underset{\sim}{R}')/2$, $\underset{\sim}{S} = \underset{\sim}{R}-\underset{\sim}{R}'$. Since (2) is already properly symmetrized with respect to interchange of $\underset{\sim}{R}$ and $\underset{\sim}{R}'$, it is often more convenient to use.

The kinetic energy density is defined as:

$$\begin{aligned}\tau(\underset{\sim}{R}) &= \frac{\hbar^2}{2m}\sum_{i=0}^{N} g_i\nabla\psi_i(\underset{\sim}{R})\cdot\nabla\psi_i(\underset{\sim}{R}) \\ &= \frac{\hbar^2}{2m}\nabla\cdot\nabla'\ \rho(\underset{\sim}{R},\underset{\sim}{R}')\Big|_{\underset{\sim}{R}=\underset{\sim}{R}'} \\ &= \frac{\hbar^2}{2m}\left(\frac{1}{4}\nabla_Q^2 - \nabla_S^2\right)\rho(\underset{\sim}{Q},\underset{\sim}{S})\Big|_{S=0}\end{aligned} \tag{3}$$

where ∇ acts only on $\underset{\sim}{R}$, ∇' acts only on $\underset{\sim}{R}'$, and ∇_Q and ∇_S act only on $\underset{\sim}{Q}$ and $\underset{\sim}{S}$ respectively.

We may also define $\tau_1(\underset{\sim}{R})$ as:

$$\tau_1(\underset{\sim}{R}) = -\frac{\hbar^2}{2m}\sum_{i=0}^{N} g_i\psi_i^*(\underset{\sim}{R})\nabla^2\psi_i(\underset{\sim}{R}) \ . \tag{4}$$

Using Green's theorem and the boundary condition on $\nabla\psi_i(\underset{\sim}{R})$, it can be shown that $\int \tau_1(\underset{\sim}{R})d^3R = \int \tau(\underset{\sim}{R})d^3R$.

The Block density matrix is given by (March et al, 1967)

$$C(\underset{\sim}{R},\underset{\sim}{R}',\beta) = \sum_{i=0}^{\infty} g_i\psi_i(\underset{\sim}{R})\psi_i(\underset{\sim}{R}')e^{-\beta\varepsilon_i} \tag{5}$$

where ε_i is the energy eigenvalue of $\psi_i(\underset{\sim}{R})$. The Block density matrix, and the transformed kinetic energy (introduced below) are used here only as a mathematical convenience to obtain the required analytical result. It is primarily because (5) is an infinite sum that we were able to obtain the result in closed form. Physically, $C(\underset{\sim}{R},\underset{\sim}{R}',\beta)$ and $\tau(\underset{\sim}{R},\beta)$ may be looked upon as a non-zero temperature generalization of (1) and (3). Since $\beta = \frac{1}{kT}$ is 40 $(\text{eV})^{-1}$ at normal temperatures, we can see that in terms of nuclear excitations of several keV, the nucleus is essentially in the zero temperature ground state. Therefore, β appears only as a parameter, which does not appear in the final result.

In analogy with (2) we find:

$$C(\underset{\sim}{Q},\underset{\sim}{S},\beta) = \sum_{i=0}^{\infty} g_i \psi_i(\underset{\sim}{Q} + \frac{\underset{\sim}{S}}{2}) \psi_i^{*}(\underset{\sim}{Q} - \frac{\underset{\sim}{S}}{2}) e^{-\beta\varepsilon_i}$$

The Block density matrix has several simple properties. The trace of $C(\underset{\sim}{R},\underset{\sim}{R}',\beta)$ is simply $Z(\beta) = \sum_{i=0}^{\infty} e^{-\beta\varepsilon_i}$, the canonical partition function. The inverse Laplace transform of $\frac{C(\underset{\sim}{R},\underset{\sim}{R}',\beta)}{\beta}$ is simply $\rho(\underset{\sim}{R},\underset{\sim}{R}',\mu)$:

$$L^{-1}[\frac{1}{\beta} C(\underset{\sim}{R},\underset{\sim}{R}',\beta);\beta\to\mu] = \sum_{i=0}^{\infty} g_i \psi_i(\underset{\sim}{R}) \psi_i^{*}(\underset{\sim}{R}') L^{-1}[\frac{e^{-\beta\varepsilon_i}}{\beta};\beta\to\mu]$$

$$= \sum_{i=0}^{\infty} g_i \psi_i(\underset{\sim}{R}) \psi_i^{*}(\underset{\sim}{R}') \theta(\mu-\varepsilon_i) \qquad (7)$$

(Abramowitz and Stegun, 1972), where $\theta(\mu-\varepsilon_i)$ is the unit step function and μ is the Fermi energy so that $\theta(\mu-\varepsilon_i) = 0$ for $i>N$, and hence (7) coincides with (1). The proof is similar for $\rho(\underset{\sim}{Q},\underset{\sim}{S})$.

The Block density matrix also obeys the Block equation:

$$H'C(\underset{\sim}{R},\underset{\sim}{R}',\beta) = -\frac{\partial}{\partial\beta} C(\underset{\sim}{R},\underset{\sim}{R}',\beta) \qquad (8)$$

as can easily be verified from equation (5). H' is the Hamiltonian operator, acting only on the $\underset{\sim}{R}'$ coordinate. The boundary condition on (8) is simply:

$$C(\underset{\sim}{R},\underset{\sim}{R}',0) = \delta(\underset{\sim}{R}-\underset{\sim}{R}') \qquad (9)$$

as can be easily seen from the fact that

$$C(\underset{\sim}{R},\underset{\sim}{R}',0) = \sum_{i=0}^{\infty} g_i \psi_i(\underset{\sim}{R}) \psi_i^*(\underset{\sim}{R}') = \delta(\underset{\sim}{R}-\underset{\sim}{R}')$$

by the condition of completeness for eigenfunctions.

We may also define the transformed kinetic energy densities:

$$\tau(\underset{\sim}{R},\beta) = \frac{\hbar^2}{2m} \sum_{i=0}^{\infty} g_i \nabla\psi_i(\underset{\sim}{R}) \cdot \nabla\psi_i^*(\underset{\sim}{R}) e^{-\beta\varepsilon_i}$$

$$= \frac{\hbar^2}{2m} \nabla\cdot\nabla' C(\underset{\sim}{R},\underset{\sim}{R}',\beta)\Big|_{R=R'} \qquad (10)$$

and

$$\tau_1(\underset{\sim}{R},\beta) = -\frac{\hbar^2}{2m} \sum_{i=0}^{\infty} g_i \psi_i^*(\underset{\sim}{R}) \nabla^2 \psi_i(\underset{\sim}{R}) e^{-\beta\varepsilon_i}$$

$$= -\frac{\hbar^2}{2m} \nabla'^2 C(\underset{\sim}{R},\underset{\sim}{R}',\beta)\Big|_{R=R'} . \qquad (11)$$

They are related to (3) and (4) respectively by:

$$L^{-1}[\frac{1}{\beta}\ \tau(\underset{\sim}{R},\beta);\beta\rightarrow\mu] = \tau(\underset{\sim}{R}) \qquad (12)$$

and

$$L^{-1}[\frac{1}{\beta}\ \tau_1(\underset{\sim}{R},\beta);\beta\rightarrow\mu] = \tau_1(\underset{\sim}{R}) \qquad (13)$$

as can be shown in a manner similar to (7).

ii) The One Dimensional Case

Below we shall derive an approximate form for the density matrix in one dimension. We begin with the exact density matrix:

$$\rho(q,s) = \sum_{i=0}^{N} g_i \psi_i(q + \frac{s}{2}) \psi_i^*(q - \frac{s}{2}) \qquad (14)$$

where q = (x+x')/2, s = s-s'.

(14) is expanded in a Taylor series of the relative coordinate to obtain:

$$\rho(q,s) = \sum_{i=1}^{N} g_i \{ \psi_i^2(q) - \frac{1}{4} ((\frac{d\psi_i(q)}{dq})^2 - \psi_i(q) \frac{d^2\psi_i(q)}{dq^2}) s^2$$
$$+ \frac{1}{16} (\frac{1}{12} \psi_i(Q) \frac{d^4\psi_i(q)}{dq^4} - \frac{1}{3} \frac{d\psi_i(q)}{dq} \frac{d^3\psi_i(q)}{dq^3} + \frac{1}{4} (\frac{d^2\psi_i(q)}{dq^2})^2) s^4 + \ldots \} \qquad (15)$$

where the wavefunction has been assumed to be real for simplicity of notation.

It is easy to see that the s^2 coefficient may be written as:

$$\frac{1}{2} \left. \frac{d^2\rho(q,s)}{ds^2} \right|_{s=0} = - \frac{1}{2} \frac{2m}{\hbar^2} (\tau(q) - \frac{1}{4} \frac{\hbar^2}{2m} \frac{d^2\rho(q)}{dq^2}) \qquad (16)$$

(see equation (3)). It is not possible to write the coefficients of s^4 and higher power in terms of $\tau(q)$ and $\frac{d^2\rho(q)}{dq^2}$ for all potentials. However, for the harmonic oscillator there exists a simple relationship between the s^2 coefficient and the higher order coefficients. To develop this relationship we derive an integral relation between the density $\rho(q)$ and the kinetic energy density $\tau(q)$ which is valid for all one dimensional single particle potentials. We then calculate the Block density matrix, $\mathcal{C}(q,s,\beta)$ explicitly for the harmonic oscillator. Upon expansion in the relative coordinate, we show that the coefficients may be written as integrals of (16). Then each coefficient contains the transformed quantities linearly, and hence the inverse transform is trivial.

The Schrödinger equation in one dimension is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_i(q)}{dq^2} + (V(q) - E_i)\psi_i(q) = 0 . \qquad (17)$$

We may differentiate (17) and multiply by $\psi_i^*(q)$ to obtain

$$-\frac{\hbar^2}{2m}\psi_i^*(q)\frac{d^3\psi_i(q)}{dq^2} + (V(q)-E_i)\psi_i^*(q)\frac{d\psi_i(q)}{dq} + \frac{dV}{dq}\psi_i^*(q)\psi_i(q) = 0 . \qquad (18)$$

If we replace $(V-E_i)\psi_i^*(q)$ by $\frac{\hbar^2}{2m}\frac{d^2\psi_i^*(q)}{dq^2}$, and add and subtract $\frac{\hbar^2}{2m}\frac{d\psi_i^*(q)}{dq}\frac{d^2\psi_i(q)}{dq^2}$, and sum over all occupied states we find:

$$\frac{\hbar^2}{2m}\sum_{i=0}^{N} g_i(-\psi_i^*(q)\frac{d^3\psi_i(q)}{dq^2} - \frac{d\psi_i^*(q)}{dq}\frac{d^2\psi_i(q)}{dq^2} + \frac{d\psi_i^*(q)}{dq}\frac{d^2\psi_i(q)}{dq^2} + \frac{d^2\psi_i^*(q)}{dq^2}\frac{d\psi_i(q)}{dq} = -\rho\frac{dV(q)}{dq} \qquad (19)$$

It is easy to see that the left hand side of (19) is simply $\frac{d}{dq}(\tau(q) + \tau_1(q))$ and hence we may integrate to obtain:

$$\tau(q) + \tau_1(q) = \int_q^\infty \rho(R) \frac{dV(R)}{dR} dR \; . \qquad (20)$$

where it is noted that $\tau(q)$ and $\tau_1(q)$ vanish at infinity. We now calculate the difference $\tau(q) - \tau_1(q)$.

$$\frac{\hbar^2}{2m} \frac{d^2\rho(q)}{dq^2} = \frac{\hbar^2}{2m} \sum_{i=0}^{N} g_i \left(\psi_i(q) \frac{d^2\psi_i^*(q)}{dq^2} + \psi_i^*(q) \frac{d^2\psi_i(q)}{dq^2} + 2 \frac{d\psi_i(q)}{dq} \frac{d\psi_i^*(q)}{dq}\right.$$

$$= 2(\tau(q) - \tau_1(q)) \; . \qquad (21)$$

We may use (20) and (21) to write:

$$\tau(q) - \frac{1}{4} \frac{\hbar^2}{2m} \frac{d^2\rho(q)}{dq^2} = \frac{1}{2} \int_q^\infty \rho(R) \frac{dV(R)}{dR} dR \; . \qquad (22)$$

$$\tau_1(q) + \frac{1}{4} \frac{\hbar^2}{2m} \frac{d^2\rho(q)}{dq^2} = \frac{1}{2} \int_q^\infty \rho(R) \frac{dV(R)}{dR} dR \; . \qquad (23)$$

It can be seen that (22) and hence (23) satisfy the virial theorem:

$$\frac{1}{2} \left\langle q \frac{dV(q)}{dq} \right\rangle = \frac{1}{2} \int_{-\infty}^{\infty} q\rho(q) \frac{dV(q)}{dq}\, dq$$

$$= \int_{-\infty}^{\infty} \frac{1}{2} \int_{q}^{\infty} \rho(R) \frac{dV(R)}{dR}\, dR\, dq$$

$$= \langle T \rangle$$

where the last step follows from the fact that $\int_{-\infty}^{\infty} \frac{d^2\rho(q)}{dq^2}\, dq = 0$ because of the boundary condition. It is to be noted that these results hold for all one dimensional single particle potentials. Furthermore, it is clear that $\tau(q)$ and $\rho(q)$ appear only linearly in the above, and hence the same relations hold for the transformed quantities $\tau(q,\beta)$ and $C(q,\beta)$.

We now calculate the Block density matrix for the harmonic oscillator. It is possible to use (8) (Feynman, 1972) but we choose to calculate it directly, using (5), since this is easier to generalize to three dimensions. The potential is:

$$V(q) = \frac{\hbar^2}{2m} \alpha^4 q^2 \tag{25}$$

where $\alpha = \sqrt{\frac{m\omega}{\hbar}}$.

The harmonic oscillator wave functions are (Landau and Lifshitz, 1977):

$$\psi_n^{H.O.}(q) = \sqrt{\frac{\alpha}{\sqrt{\pi}2^n n!}}\, e^{-\alpha^2 q^2/2} H_n(\alpha q)$$

corresponding to the energy eigenvalue $\varepsilon_n = (n + \frac{1}{2})\hbar\omega$.

Then formally we may write:

$$C^{H.O.}(x,x',\beta) = \frac{\alpha}{\sqrt{\pi}}\, e^{-\frac{\alpha^2}{2}(x^2+x'^2)}\, e^{-\frac{\beta\hbar\omega}{2}} \sum_{n=0}^{\infty} \frac{H_n(\alpha x)H_n(\alpha x')}{2^n n!}(e^{-\beta\hbar\omega})^n \quad (27)$$

where the factor $e^{-\frac{\beta\hbar\omega}{2}}$ comes from the zero point energy. The generating function (Magnus et al, 1966)

$$\sum_{n=0}^{\infty} \frac{H_n(x)H_n(x')}{2^n n!} y^n = \frac{1}{\sqrt{1-y^2}} \exp\left(x'^2 - \frac{(x'-xy)^2}{1-y^2}\right) \quad (28)$$

where we identify $e^{-\beta\hbar\omega}$ with y, may be used to write (27) in closed form.

$$C^{H.O.}(x,x',\beta) = \frac{\alpha e^{-\beta\hbar\omega/2}}{\sqrt{\pi(1-e^{-2\beta\hbar\omega})}}\, e^{-\frac{\alpha^2}{2}(x^2+x'^2)} \exp\left(\alpha^2\left(x'^2 - \frac{(x'-xe^{-\beta\hbar\omega})^2}{1-e^{-2\beta\hbar\omega}}\right)\right) \quad (29)$$

(29) may be rearranged into a more convenient form using hyperbolic trigonometric functions to obtain:

$$C^{H.O.}(x,x',\beta) = \frac{\alpha}{\sqrt{2\pi\sinh(\beta\hbar\omega)}} \exp\left(-\frac{\alpha^2}{2}(x^2+x'^2)\coth(\beta\hbar\omega) - 2xx'\operatorname{csch}(\beta\hbar\omega)\right). \quad (30)$$

Using the identity $\tanh(\frac{Z}{2}) = \coth(Z) - \operatorname{csch}(Z)$ we write the diagonal Block density matrix.

$$C^{H.O.}(x,\beta) = \frac{\alpha}{\sqrt{2\pi\sinh(\beta\hbar\omega)}} \exp\left(-\alpha^2 x^2 \tanh\left(\frac{\beta\hbar\omega}{2}\right)\right) \quad (31)$$

This agrees with the result obtained by Feynman (Feynman, 1972). We may write (30) in terms of the centre of mass and relative coordinates to obtain:

$$C^{H.O.}(q,s,\beta) = \frac{\alpha}{\sqrt{2\pi\sinh(\beta\hbar\omega)}} \exp(-\alpha^2 q^2 \tanh(\beta\hbar\omega/2)) \exp(-\frac{\alpha^2 s^2}{4} \coth(\beta\hbar\omega/2)) \tag{32}$$

The reason for using the Block density matrix rather than the density matrix is now readily apparent. Not only does it allow one to write the matrix in closed form, it also gives a complete separation of the matrix into a multiple of the diagonal matrix times the off diagonal elements. This makes an expansion in s rather easy. (32) shows explicitly the invariance under interchange of x and x' and thus, will have a Taylor series in s^2, not simply s.

Using (10) and (32) we may now calculate $\tau^{H.O.}(q,\beta)$.

$$\tau^{H.O.}(q,\beta) = \frac{\hbar^2}{2m} (\alpha^4 \tanh^2(\frac{\beta\hbar\omega}{2}) q^2 + \alpha^2 \operatorname{csch}(\beta\hbar\omega)) C^{H.O.}(q,\beta) \tag{33}$$

where the identity $\frac{1-\tanh^2(x/2)}{2\tanh(x/2)} = \operatorname{csch}(x)$ has been used. Since

$$\frac{1}{4} \frac{d^2 C^{H.O.}(q,\beta)}{dq^2} = (\alpha^4 \tanh^2(\frac{\beta\hbar\omega}{2}) q^2 - \frac{\alpha^2}{2} \tanh(\frac{\beta\hbar\omega}{2})) C^{H.O.}(q,\beta)$$

we have

$$\tau^{H.O.}(q,\beta) - \frac{1}{4} \frac{\hbar^2}{2m} \frac{d^2 C^{H.O.}(q,\beta)}{dq^2} = \frac{\hbar^2}{2m} \frac{\alpha^2}{2} \coth(\frac{\beta\hbar\omega}{2}) C^{H.O.}(q,\beta). \tag{34}$$

We may use the integral: $\int_q^\infty x e^{-ax^2} dx = \frac{1}{2a} e^{-aq^2}$ and write $x = \frac{1}{2\alpha^4} \frac{2m}{\hbar^2} \frac{dV(x)}{dx}$ to verify (22) explicitly for the harmonic oscillator.

$$\frac{1}{2\alpha^4} \frac{2m}{\hbar^2} \int_q^\infty \frac{\alpha}{\sqrt{2\pi \sinh(\beta\hbar\omega)}} \exp(-\alpha^2 x^2 \tanh(\frac{\beta\hbar\omega}{2})) \frac{dV(x)}{dx}\, dx \; .$$

$$= \frac{1}{2\alpha^2} \coth(\frac{\beta\hbar\omega}{2}) \frac{\alpha}{\sqrt{2\pi \sinh(\beta\hbar\omega)}} \exp(-\alpha^2 q^2 \tanh(\frac{\beta\hbar\omega}{2})) \tag{35}$$

which, when compared with (34) shows:

$$\frac{1}{2} \int_q^\infty C^{H.O.}(x,\beta) \frac{dV(x)}{dx}\, dx = \tau^{H.O.}(q,\beta) - \frac{1}{4} \frac{\hbar^2}{2m} \frac{d^2 C^{H.O.}(q,\beta)}{dq^2} \; . \tag{36}$$

Upon repeated integration, we find:

$$(\frac{2m}{\hbar^2})^n \int_q^\infty \int_{x_1}^\infty \cdots \int_{x_{n-1}}^\infty C^{H.O.}(x_n,\beta) \frac{dV(x_n)}{dx_n} dx_n \cdots \frac{dV(x_1)}{dx_1} dx_1$$

$$= 2(\frac{2m}{\hbar^2})^n \int_q^\infty \cdots \int_{x_1}^\infty \cdots \int_{x_{n-2}}^\infty (\tau^{H.O.}(x_{n-1},\beta) -$$

$$- \frac{1}{4} \frac{\hbar^2}{2m} \frac{d^2 C^{H.O.}(x_{n-1},\beta)}{dx_{n-1}^2}) \frac{dV(x_{n-1})}{dx_{n-1}} dx_{n-1} \cdots \frac{dV(x_1)}{dx_1} dx_1$$

$$= \alpha^{2n} \coth^n(\frac{\beta\hbar\omega}{2}) C^{H.O.}(q,\beta) \; . \tag{37}$$

If we expand (32) in a Taylor Series, expand about s=0 and compare with (37) we see that:

$$C^{H.O.}(q,s,\beta) = C^{H.O.}(q,\beta) - \frac{\alpha^2}{4}\coth\left(\frac{\beta\hbar\omega}{2}\right)(C^{H.O.}(q,\beta)s^2$$

$$+ \frac{\alpha^4}{32}\coth^2\left(\frac{\beta\hbar\omega}{2}\right)C^{H.O.}(q,\beta)s^4 + \cdots$$

$$+ (-)^n \frac{\alpha^{2n}}{4^n n!}\coth^n\left(\frac{\beta\hbar\omega}{2}\right)C^{H.O.}(q,\beta)s^{2n} + \cdots$$

$$= C^{H.O.}(q,\beta) - \frac{1}{2}\frac{2m}{\hbar^2}\left(\tau^{H.O.}(q,\beta) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2C^{H.O.}(q,\beta)}{dq^2}\right)s^2 +$$

$$+ \frac{1}{16}\left(\frac{2m}{\hbar^2}\right)^2 \int_q^\infty \left(\tau^{H.O.}(x,\beta) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2C^{H.O.}(x,\beta)}{dx^2}\right)\frac{dV}{dx}\,dx$$

$$\cdot\, s^4 + \cdots + (-)^n \frac{2}{4^n n!}\left(\frac{2m}{\hbar^2}\right)^n \int_q^\infty\int_{x_1}^\infty \cdots \int_{x_{n-2}}^\infty \left(\tau^{H.O.}(x_{n-1},\beta)\right.$$

$$\left. - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2C^{H.O.}(x_{n-1},\beta)}{dx_{n-1}^2}\right)\frac{dV}{dx_{n-1}}\,dx_{n-1}\cdots\frac{dV}{dx_1}\,dx_1$$

$$\cdot\, s^{2n} + \cdots . \tag{38}$$

Since all the transformed quantities in (38) appear linearly, it is simple to Laplace invert (38) to obtain the expression for the density matrix with the sharp Fermi surface.

$$\rho^{H.O.}(q,s,\mu) = \rho^{H.O.}(q,\mu) - \frac{1}{2}\frac{2m}{\hbar^2}\left(\tau^{H.O.}(q,\mu) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2\rho^{H.O.}(q,\mu)}{dq^2}\right)s^2$$

$$+ \frac{1}{16}\left(\frac{2m}{\hbar^2}\right)^2 \int_q^\infty \left(\tau^{H.O.}(x,\mu) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2\rho^{H.O.}(x,\mu)}{dx^2}\right)\frac{dV(x)}{dx}\,dx\,s^4 + \cdots$$

$$+ (-)^n \frac{2}{4^n n!}\left(\frac{2m}{\hbar^2}\right)^n \int_q^\infty \int_{x_1}^\infty \cdots \int_{x_{n-2}}^\infty \left(\tau^{H.O.}(x_{n-1},\mu) -\right.$$

$$\left. - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2\rho^{H.O.}(x_{n-1},\mu)}{dx_{n-1}^2}\right)\frac{dV(x_{n-1})}{dx_{n-1}}\,dx_{n-1}\cdots\frac{dV(x_1)}{dx_1}\,dx_1$$

$$\cdot\, s^{2n} + \cdots \quad . \qquad (39)$$

As mentioned earlier, β does not appear in the final result. There is a parameter μ, which is necessary because of (7). However, μ, which is the Fermi energy, is fixed by N, the number of particles in the potential.

(39) is also reproduced for the linear potential $V = kx$ and quadratic potentials of the form $V = a+bx+cx^2$ as is shown in Appendix A. This leads us to believe that the density above will be good wherever higher than second derivatives of the potential are small. This should not be surprising since it is known (de Shalit and Feshbach, 1974) that harmonic oscillator wavefunctions are reasonably good in the interior of the nucleus, but rather poor in the nuclear surface. However, if one looks at smooth one-body nuclear potentials, such as the Woods-Saxon, one finds that within the interior of the

nucleus it has very small high order derivatives, and it is not until one gets close to the nuclear tail that the high order derivatives become large with respect to the low order derivatives.

The accuracy of (39) is checked in a model potential whose eigenfunctions are known analytically (see chapter 3). It is seen that (39) is reasonably good even when higher than second derivatives are not necessarily small. The accuracy is also compared to other approximations such as the Campi-Bouyssy and Negele-Vautherin, and (39) is found to be comparable in accuracy to these expansions.

iii) The Three Dimensional Case

In 3 dimensions we may write the density matrix as:

$$\rho(\underset{\sim}{Q},\underset{\sim}{S}) = \sum_{i=0}^{N} g_i \psi_i(\underset{\sim}{Q} + \tfrac{\underset{\sim}{S}}{2})\psi_i^{*}(\underset{\sim}{Q} - \tfrac{\underset{\sim}{S}}{2}).$$

If we expand in a Taylor series of the relative coordinate $\underset{\sim}{S}$ we find:

$$\begin{aligned}\rho(\underset{\sim}{Q},\underset{\sim}{S}) = \sum_{i=0}^{N} g_i \{ & \psi_i^{*}(\underset{\sim}{Q})\psi_i(\underset{\sim}{Q}) + \frac{1}{4}\,(\psi_i^{*}(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\nabla)^2\psi_i(\underset{\sim}{Q}) \\ & - \underset{\sim}{S}\cdot\nabla\psi_i^{*}(\underset{\sim}{Q})\,\underset{\sim}{S}\cdot\nabla\psi_i(\underset{\sim}{Q})) + \frac{1}{192}\,(\psi_i^{*}(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\nabla)^4\psi_i(\underset{\sim}{Q}) \\ & - 4(\underset{\sim}{S}\cdot\nabla)\psi_i^{*}(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\nabla)^3\psi_i(\underset{\sim}{Q}) + 3(\underset{\sim}{S}\cdot\nabla)^2\psi_i^{*}(\underset{\sim}{Q}) \\ & (\underset{\sim}{S}\cdot\nabla)^2\psi_i(\underset{\sim}{Q})) + \cdots\} \, . \qquad (40)\end{aligned}$$

The angle average of (40) is given in appendix B.

$$\rho(\underset{\sim}{Q},\underset{\sim}{S}) = \rho(\underset{\sim}{Q}) - \frac{1}{12}\sum_i g_i\{\nabla\psi_i^*(\underset{\sim}{Q})\cdot\nabla\psi_i(\underset{\sim}{Q}) - \psi_i^*(\underset{\sim}{Q})\nabla^2\psi_i(\underset{\sim}{Q})\}S^2$$

$$+ \frac{1}{960}\sum_i g_i\{\psi_i^*(\underset{\sim}{Q})\nabla^4\psi_i(\underset{\sim}{Q}) - 4\nabla\psi_i^*\cdot\nabla\nabla^2\psi_i(\underset{\sim}{Q}) + \nabla^2\psi_i^*(\underset{\sim}{Q})\nabla^2\psi_i(\underset{\sim}{Q})$$

$$+ 2\nabla\nabla\psi_i^*(\underset{\sim}{Q}):\nabla\nabla\psi_i(\underset{\sim}{Q})\}S^4 + \ldots \qquad (40a)$$

where the last term in the fourth order co-efficient is defined in appendix B. The S^2 coefficient may be written as

$$-\frac{1}{12}\sum_{i=1}^{N} g_i(\nabla\psi_i^*(\underset{\sim}{Q})\cdot\nabla\psi_i(\underset{\sim}{Q}) - \psi_i^*(\underset{\sim}{Q})\nabla^2\psi_i(\underset{\sim}{Q}))$$

$$= -\frac{1}{6}\frac{2m}{\hbar^2}(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})) \qquad (41)$$

which is the three dimensional analogue of (16). It is also easy to see the analogous relation to (21) holds in 3 dimensions.

$$\tau(Q) - \tau_1(\underset{\sim}{Q}) = \frac{1}{2}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q}) \; . \qquad (42)$$

However, it is not possible, in general, to reproduce equation (20) for all potentials in three dimensions. The reason is that in going from (18) to (19) (in the spherically symmetric case), we would need the following relation to hold:

$$-\frac{\hbar^2}{2m}\sum_{i=0}^{N} g_i(\psi_i^*(\underset{\sim}{Q})\nabla\nabla^2\psi_i(\underset{\sim}{Q})+\nabla\psi_i^*(\underset{\sim}{Q})\nabla^2\psi_i(\underset{\sim}{Q}))+\frac{\hbar^2}{2m}\sum_{i=0}^{\infty} g_i(\nabla\psi_i^*(\underset{\sim}{Q})\nabla^2\psi_i(\underset{\sim}{Q}) +$$

$$+ \nabla^2\psi_i^*(\underset{\sim}{Q})\nabla\psi_i(\underset{\sim}{Q})$$

$$= \nabla(\tau(\underset{\sim}{Q}) + \tau_1(\underset{\sim}{Q})) \qquad (43)$$

which is a very restrictive condition. But it is possible to show explicitly that the three dimensional harmonic oscillator obeys a relation analogous to (20). This shows that (43) is a sufficient, but not necessary condition that relation (44) is satisfied.

$$\tau'(\underset{\sim}{Q}) = \frac{3}{2}\int_{Q}^{\infty} \rho(\underset{\sim}{R})\, \frac{dV(\underset{\sim}{R})}{dR}\, dR + \frac{1}{4}\,\frac{\hbar^{2}}{2m}\,\nabla^{2}\rho(\underset{\sim}{Q}) \; . \qquad (44)$$

An integration by parts shows that:

$$\frac{1}{2}\langle \underset{\sim}{Q}\cdot\nabla V\rangle = \frac{1}{2}\,4\pi \int_{0}^{\infty} Q^{3}\, \frac{dV(\underset{\sim}{Q})}{dQ}\, \rho(\underset{\sim}{Q})\,dQ$$

$$= 4\pi \int_{0}^{\infty} \frac{3}{2}\int_{Q}^{\infty} \rho(\underset{\sim}{R})\, \frac{dV(\underset{\sim}{R})}{dR}\, dR\; Q^{2}dQ$$

$$= \langle T'\rangle \qquad (45)$$

where we have assumed $\tau(\underset{\sim}{Q})$ and $\rho(\underset{\sim}{Q})$ to be spherically symmetric and we have used the boundary condition to see that

$$\int \nabla^{2}\rho(\underset{\sim}{Q})\,d^{3}Q = 0.$$

Thus a kinetic energy density defined by (44) satisfies the virial theorem. It will be shown below that the three dimensional isotropic harmonic oscillator does satisfy (44).

For a separable potential $V(\underset{\sim}{R}) = V(x) + V(y) + V(z)$ the wavefunctions separate into products of wavefunctions of each coordinate. Hence, the Block density matrix for such a potential is simply:

$$C(\underset{\sim}{R},\underset{\sim}{R}',\beta) = \prod_{i=1}^{3} C(x_i,x_i',\beta) \quad . \tag{46}$$

Then we may use (30) to write:

$$C^{H.O.}(\underset{\sim}{R},\underset{\sim}{R}',\beta) = \left(\frac{\alpha^2}{2\pi\sinh(\beta\hbar\omega)}\right)^{3/2} \exp\left(-\frac{\alpha^2}{2}\left((R^2+R'^2)\coth(\beta\hbar\omega) - 2\underset{\sim}{R}\cdot\underset{\sim}{R}'\operatorname{csch}(\beta\hbar\omega)\right)\right) \tag{47}$$

which may be written in the centre of mass system as:

$$C^{H.O.}(\underset{\sim}{Q},\underset{\sim}{S},\beta)=\left(\frac{\alpha^2}{2\pi\sinh(\beta\hbar\omega)}\right)^{3/2} \exp\left(-\alpha^2Q^2\tanh\left(\frac{\beta\hbar\omega}{2}\right)\right)\exp\left(-\frac{\alpha^2S^2}{4}\coth\left(\frac{\beta\hbar\omega}{2}\right)\right) . \tag{48}$$

Using (48) and (10) we may calculate the kinetic energy density.

$$\tau^{H.O.}(\underset{\sim}{Q},\beta) = \frac{\hbar^2}{2m}\left(\frac{3}{2}\alpha^2\coth\left(\frac{\beta\hbar\omega}{2}\right) + \frac{3}{2}\alpha^2\tanh\left(\frac{\beta\hbar\omega}{2}\right) + \alpha^4Q^2\tanh^2\left(\frac{\beta\hbar\omega}{2}\right)\right)C^{H.O.}(\underset{\sim}{Q},\beta) \tag{49}$$

and hence :

$$\tau^{H.O.}(\underset{\sim}{Q},\beta) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2 C^{H.O.}(\underset{\sim}{Q},\beta) = \frac{3}{2}\frac{\hbar^2}{2m}\alpha^2\coth(\frac{\beta h\omega}{2})C^{H.O.}(\underset{\sim}{Q},\beta)$$

$$= \frac{3}{2}\int^{\infty} C^{H.O.}(\underset{\sim}{R},\beta)\ \frac{dV(R)}{dR}\ dR \qquad (50)$$

(see equation (35)).

Therefore, we have shown explicitly that the harmonic oscillator kinetic energy density may be written in the same form as (44). It is then easy to show that a relation similar to (37) also holds in 3 dimensions.

$$\alpha^{2n}\coth^n(\beta h\omega/2)C^{H.O.}(\underset{\sim}{Q},\beta) = \frac{2}{3}\ (\frac{2m}{\hbar^2})^n \int_{Q}^{\infty}\int_{R_1}^{\infty}\cdots\int_{R_{n-2}}^{\infty} (\tau^{H.O.}(\underset{\sim}{R}_{n-1},\beta) -$$

$$- \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2 C^{H.O.}(\underset{\sim}{R}_{n-1},\beta))\ \frac{dV}{dR_{n-1}}\ dR_{n-1}\cdots\frac{dV}{dR_1}\ dR_1 \qquad (51)$$

To generalize (38) to 3 dimensions we use (51) to write:

$$C^{H.O.}(\underset{\sim}{Q},\underset{\sim}{S},\beta) = C^{H.O.}(\underset{\sim}{Q},\beta) - \frac{1}{6}\ \frac{2m}{\hbar^2}\ (\tau^{H.O.}(\underset{\sim}{Q},\beta) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2 C^{H.O.}(\underset{\sim}{Q},\beta))S^2$$

$$+ \frac{1}{48}\ (\frac{2m}{\hbar^2})^2 \int^{\infty} (\tau^{H.O.}(\underset{\sim}{R},\beta) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2 C^{H.O.}(\underset{\sim}{R},\beta))\frac{dV}{dR}dR\ S^4\cdots$$

$$+ \frac{2}{3.4^{n}n!}\ (\frac{2m}{\hbar^2})^n \int_{Q}^{\infty}\cdots\int_{R_{n-2}}^{\infty} (\tau^{H.O.}(\underset{\sim}{R}_{n-1},\beta) -$$

$$- \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2 C^{H.O.}(\underset{\sim}{R}_{n-1},\beta))\ \frac{dV}{dR_{n-1}}\ dR_{n-1}\cdots\frac{dV}{dR_1}\ dR_1\ S^{2n} + \cdots.$$

(52)

Again, all the transformed quantities appear linearly in (52). Hence we may Laplace invert (52) to get the sharp Fermi surface result:

$$\begin{aligned}
\rho^{H.O.}(\underset{\sim}{Q},S) = {} & \rho^{H.O.}(\underset{\sim}{Q}) - \frac{1}{6}\frac{2m}{\hbar^2}\left(\tau^{H.O.}(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho^{H.O.}(\underset{\sim}{Q})\right)S^2 \\
& + \frac{1}{48}\left(\frac{2m}{\hbar^2}\right)^2 \int_Q^\infty \left(\tau^{H.O.}(\underset{\sim}{R}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho^{H.O.}(\underset{\sim}{R})\right)\frac{dV}{dR}\,dR\;S^4 + \cdots \\
& + \frac{2}{3.4^n n!}\left(\frac{2m}{\hbar^2}\right)^n \int_Q^\infty \cdots \int_{R_{n-2}}^\infty \left(\tau^{H.O.}(\underset{\sim}{R}_{n-1}) - \right. \\
& \left. - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho^{H.O.}(\underset{\sim}{R}_{n-1})\right)\frac{dV}{dR_{n-1}}\,dR_{n-1}\cdots\frac{dV}{dR_1}\,dR_1\;S^{2n} + \cdots
\end{aligned} \tag{53}$$

(53) is the form of the density matrix expansion which we propose to use. It is important to realize that this derivation depends crucially on (51). It was not possible to Laplace invert a Taylor series expansion in $\underset{\sim}{S}$ of (48) until the coefficients were "linearized". The sacrifice one makes for this is nonlocality in the expansion coefficients.

Other density matrix expansions are written in terms of local coefficients. To compare them with (53), we evaluate (53) and the other expansions in a local gradient approximation. This is done in chapter 2 to show the relation between our work and other approaches.

In the third chapter we use (53) to evaluate the density matrix. These are compared to exact calculations and to calculations using other approximations. It is shown that (53) is reasonably accurate.

CHAPTER 2

CONNECTION WITH ALTERNATIVE APPROACHES

i) Alternative Forms for the Density Matrix

Several forms have been proposed as approximations to the nuclear density matrix. Negele and Vautherin (1972) expand the exact density matrix in a basis of spherical Bessel functions. This has the advantage that the first order term is the Slater mixed density which is exact for uniform nuclear matter, with all higher order terms vanishing in uniform nuclear matter. The other terms are then a measure of the departure of the density matrix for finite nuclear matter from that of uniform nuclear matter.

As with a Taylor series expansion, an expansion in Bessel functions is exact up to infinite order. When truncated at a finite order, and expanded in a Taylor series in S, it reproduces the exact Taylor series expansion up to that order, but in essence corresponds to having undetermined coefficients in higher order powers of S. Thus, when Negele and Vautherin truncate the Bessel function expansion after the first correction term, it reproduces the exact Taylor series expansion up to S^2, with the coefficients of S^4 and higher terms undetermined

(Negele and Vautherin, 1972). It is with the density matrix given by (1) that we shall make the connection to the harmonic approximation, to see how this truncated expansion reproduces the higher powers of a Taylor series expansion.

$$\rho^{N.V.}(\underset{\sim}{Q},\underset{\sim}{S}) = \rho(\underset{\sim}{Q})\hat{j}_1(k_F S) + \frac{1}{6}\hat{j}_3(k_F S)\left[\frac{2m}{\hbar^2}\left(\frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q}) - \tau(\underset{\sim}{Q})\right) + \frac{3}{5}k_F{}^2\rho(\underset{\sim}{Q})\right]S^2 + \cdots \qquad (1)$$

where k_F is the Fermi momentum in the local density approximation defined by: $k_F = (3\pi^2\rho(\underset{\sim}{Q}))^{1/3}$; and $\hat{j}_n(x) = \frac{(2n+1)!!}{x^n} j_n(x)$, $j_n(x)$ being the spherical Bessel function of order n.

Campi and Bouyssy (1978) realized that by a change in the definition of k, the second term in (1) vanishes, thus leaving a Slater-like form for the density matrix. As pointed out in their paper, this "effective" momentum may be seen as a convergence producing factor, even though the full expansion does not depend on the definition of k. Therefore, if we define k to be:

$$\hat{k} = \left(\frac{5}{3\rho(\underset{\sim}{Q})}\left(\frac{2m}{\hbar^2}\right)\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right)\right)^{1/2} \qquad (2)$$

then (1) becomes:

$$\rho^{C.B.}(\underset{\sim}{Q},\underset{\sim}{S}) = \rho(\underset{\sim}{Q})\hat{j}_1(\hat{k}S) \ . \qquad (3)$$

Both of these forms have been looked at numerically, in this thesis (see chapter 3), and elsewhere (Bhaduri and Sprung, 1978; Campi and Bouyssy, 1978). It appears that $\rho^{C.B.}(\underset{\sim}{Q},\underset{\sim}{S})$

tends to give better values for the matrix elements. In model calculations $\rho^{C.B.}(\underset{\sim}{Q},\underset{\sim}{S})$ tends to be more accurate in the tail and less accurate in the interior than $\rho^{N.V.}(\underset{\sim}{Q},\underset{\sim}{S})$ when they are compared to the exact density matrix (Campi and Bouyssy, 1978).

A third form has been proposed by Jennings (Jennings, 1978). Based upon a semi-classical expansion, it is given in (4).

$$
\begin{aligned}
\rho^{J}(\underset{\sim}{Q},\underset{\sim}{S}) = \{ & \rho_{S.C.}\hat{j}_1(kS) + \frac{5}{2k^2}\left[\frac{2m}{\hbar^2}\left(\frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho_{S.C.} - \tau_{S.C.}\right) + \frac{3}{5}k^2\rho_{S.C.}\right. \\
& \left. + \frac{1}{24\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(\lambda-V)^{1/2}\left(\nabla^2 V - \frac{3(\underset{\sim}{S}\cdot\nabla)^2 V}{S^2}\right)\right] j_2(kS) \\
& - \frac{1}{24\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}(\lambda-V)^{-1/2}\left[\nabla^2 V - \frac{9}{4}\frac{(\nabla V)^2}{\lambda-V} - 5\frac{(\underset{\sim}{S}\cdot\nabla)^2 V}{S^2} V\right] kS j_3(kS) \\
& - \frac{1}{48\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}(\lambda-V)^{1/2}\left[\frac{1}{2}\frac{(\nabla V)^2}{(\lambda-V)} + \frac{(\underset{\sim}{S}\cdot\nabla)^2}{S^2}\right] k^2S^2 j_4(kS)\}\,\theta(\lambda-V) \qquad (4)
\end{aligned}
$$

where λ is the semi-classical fermi energy which is determined by integrating the semi-classical density of states; and $\rho_{S.C.}$, $\tau_{S.C.}$ and k are given by gradient expansions (Jennings, 1976). Since this result is semi-classical, it is valid only to the turning point where $V(\underset{\sim}{Q}_{T.P.}) = \lambda$. Hence the step function cuts off the density at the turning point.

In order to compare (4) with other approaches, we must angle average it over the directions of $\underset{\sim}{S}$. When this is done we obtain:

$$\overline{\rho^{J}}(\underset{\sim}{Q},\underset{\sim}{S}) = \{\rho_{S.C.}\hat{j}_1(kS) + \frac{5}{2k^2}\,[\frac{2m}{\hbar^2}\,(\frac{1}{4}\,\frac{\hbar^2}{2m}\,\nabla^2\rho_{S.C.} - \tau_{S.C.}) + \frac{3}{5}\,k^2\rho_{S.C.}]\hat{j}_2(kS)$$

$$+ \frac{1}{24\pi^2}\,(\frac{2m}{\hbar^2})^{1/2}[\frac{2}{3}\,\frac{\nabla^2 V}{\sqrt{\lambda-V}} + \frac{9}{4}\,\frac{(\nabla V)^2}{(\lambda-V)^{3/2}}]kSj_3(kS)$$

$$- \frac{1}{48\pi^2}\,(\frac{2m}{\hbar^2})^{1/2}[\frac{1}{2}\,\frac{(\nabla V)^2}{(\lambda-V)^{3/2}} + \frac{1}{3}\,\frac{\nabla^2 V}{\sqrt{\lambda-V}}]k^2S^2j_4(kS)\}\theta(\lambda-V). \quad (5)$$

We reproduce the semi-classical expression used (Jennings, 1976), up to the first order correction term, since (4) was derived up to this order.

$$\rho_{S.C.}(\underset{\sim}{R}) = (\frac{2m}{\hbar^2})^{3/2}\cdot\frac{1}{3\pi^2}\,(\lambda-V(R))^{3/2} - (\frac{2m}{\hbar^2})^{1/2}\,\frac{1}{24\pi^2}\,\{\frac{(\nabla V(R))^2}{4(\lambda-V(R))^{3/2}} + \frac{\nabla^2 V(R)}{\sqrt{\lambda-V(R)}}\} \quad (6)$$

$$\tau_{S.C.}(\underset{\sim}{R}) = (\frac{2m}{\hbar^2})^{3/2}\,\frac{1}{5\pi^2}\,(\lambda-V(\underset{\sim}{R}))^{5/2} - (\frac{2m}{\hbar^2})^{1/2}\,\frac{1}{8\pi^2}\,\{\frac{3}{4}\,\frac{(\nabla V(R))^2}{\sqrt{\lambda V-(R)}} -$$

$$- \frac{5}{3}\,\sqrt{\lambda-V(R)}\,\nabla^2 V(R)\} \quad (7)$$

$$k(\underset{\sim}{R}) = \sqrt{\frac{2m}{\hbar^2}\,(\lambda-V(\underset{\sim}{R}))} \quad (8)$$

$$\tau_{S.C.} - \frac{1}{4}\,\frac{\hbar^2}{2m}\,\nabla^2\rho_{S.C.} = (\frac{2m}{\hbar^2})^{3/2}\cdot\frac{1}{5\pi^2}\,(\lambda-V(R))^{5/2}$$

$$+ (\frac{2m}{\hbar^2})^{1/2}\,\frac{1}{8\pi^2}\{\frac{1}{4}\,\frac{(\nabla V(R))^2}{\sqrt{\lambda-V(R)}} - \frac{2}{3}\,\sqrt{\lambda-V(R)}\,\nabla^2 V(R)\} \quad (9)$$

where the above are all multiplied by the step function $\theta(\lambda - V(R))$. The first term in each of the above is the Thomas-Fermi expression.

While all three expansions above are local, our expansion (1.53) contains non-local coefficients. In order to show the relationship between our approach and the three above we use the semiclassical expressions above to evaluate the integrals in (1.53). First we expand (1), (3) and (5) in a power series of S^2 up to order S^6:

$$\begin{aligned}\rho^{\mathrm{N.V.}}(\underset{\sim}{Q},\underset{\sim}{S}) &= \rho(\underset{\sim}{Q}) - \frac{1}{6}\left(\frac{2m}{\hbar^2}\right)\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right)S^2 \\ &+ \left(\frac{k_F^2}{108}\frac{2m}{\hbar^2}\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right) - \frac{k_F^4}{504}\rho(\underset{\sim}{Q})\right)S^4 \\ &- \left(\frac{k_F^4}{4752}\left(\frac{2m}{\hbar^2}\right)\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right) - \frac{k_F^6}{16{,}632}\rho(\underset{\sim}{Q})\right)S^6 \qquad (10)\end{aligned}$$

$$\begin{aligned}\rho^{\mathrm{C.B.}}(\underset{\sim}{Q},\underset{\sim}{S}) &= \rho(\underset{\sim}{Q}) - \frac{1}{6}\left(\frac{2m}{\hbar^2}\right)\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right)S^2 \\ &+ \frac{5}{504}\left(\frac{2m}{\hbar^2}\right)^2\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right)^2/\rho(\underset{\sim}{Q})S^4 \\ &- \frac{25}{81{,}649}\left(\frac{2m}{\hbar^2}\right)^3\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right)^3/(\rho(\underset{\sim}{Q}))^2S^6 \qquad (11)\end{aligned}$$

$$\begin{aligned}\overline{\rho_J(\underset{\sim}{Q},\underset{\sim}{S})} &= \Big\{\rho(\underset{\sim}{Q}) - \frac{1}{6}\frac{2m}{\hbar^2}\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right)S^2 \\ &+ \frac{1}{24}\Big[\frac{2k^2}{7}\frac{2m}{\hbar^2}\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right) - \frac{3}{35}k^4\rho(\underset{\sim}{Q}) + \left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{k^4}{105\pi^2}\,\frac{2}{3}\,\frac{\nabla^2 V}{\sqrt{\lambda - V}} \\ &+ \frac{9}{4}\frac{(\nabla V)^2}{(\lambda - V)^{3/2}}\Big]S^4 - \frac{1}{432}\Big[\frac{k^4}{7}\frac{2m}{\hbar^2}\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q}) - \frac{2k^6}{35}\rho(\underset{\sim}{Q})\right. \\ &+ \frac{k^6}{105\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\left(\frac{\nabla^2 V}{\sqrt{\lambda - V}} + \frac{11}{4}\frac{(\nabla V)^2}{(\lambda - V)^{3/2}}\right)\Big]S^6\Big\}\theta(\lambda - V) \qquad (12)\end{aligned}$$

It is clear that all of the above expressions, as well as (1.53) agree with the exact expression up to order S^2. It is only in the S^4 and higher power coefficients that they differ. Therefore we will show the relation between our approach and the others for the higher coefficients. We do this first by evaluating the integrals in (1.53) using (6) through (9). This shall show that within the semi-classical formalism, our approach reduces to Jennings' approach. Next we use the connection between (1) and (5) to infer the relationship between our approach, and that of Negele and Vautherin. Finally, we evaluate the integrals in (1.53) within the Thomas-Fermi approximation and show that our approach then reduces to that of Campi and Bouyssy.

ii) <u>The Connection with Jennings' Approach</u>

The appropriate expressions for ρ, τ and k are found in equations (6) through (9). We use them to evaluate the S^4 coefficient in our harmonic approximation, (1.53). Omitting the factor: $\frac{1}{48}\left(\frac{2m}{\hbar^2}\right)^2$ we have:

$$S4^{H.O.} = \int_{Q}^{\infty} \left(\tau(r) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla\rho^2(r)\right)\frac{dV}{dr}\,dr \,. \qquad (13)$$

From (9) we have:

$$S4^{H.O.} = [\frac{(\frac{2m}{\hbar^2})^{3/2}}{5\pi^2} \int_Q^\infty (\lambda-V)^{5/2} \frac{dV}{dr}\, dr + \frac{(\frac{2m}{\hbar^2})^{1/2}}{8\pi^2} \int_Q^\infty (\frac{1}{4} \frac{(\nabla V)^2}{\sqrt{\lambda-V}} -$$

$$- \frac{2}{3} \sqrt{\lambda-V}\ \nabla^2 V)\ \frac{dV}{dr}\, dr]\, \theta(\lambda-V) \quad . \qquad (14)$$

We may note that $\frac{dV}{dr}\ dr = dV$ and also use:

$$- \frac{1}{2\ \frac{dV}{dr}} \frac{d}{dr} \{\sqrt{\lambda-V}\ (\frac{dV}{dr})^2\} = \frac{(\frac{dV}{dr})^2}{4\sqrt{\lambda-V}} - \sqrt{\lambda-V}\ \frac{d^2V}{dr^2} \ .$$

We also exploit the fact that we are assuming higher gradients of V are small so that $\nabla^2 V$ is a constant, and it is equal to $3\ \frac{d^2V}{dr^2}$ as is true for the harmonic oscillator. Then (14) may be integrated to give:

$$S4^{H.O.} = ((\frac{2m}{\hbar^2})^{3/2} \frac{2}{35\pi^2}\ (\lambda-V)^{7/2} + (\frac{2m}{\hbar^2})^{5/2} (\frac{1}{16\pi^2}\ \sqrt{\lambda-V}(\nabla V)^2 -$$

$$- \frac{1}{36\pi^2}\ (\lambda-V)^{3/2} \nabla^2 V))\, \theta(\lambda-V) \qquad (15)$$

We may re-arrange (15) using (6), (7), (8) and (9) and include the factor $\frac{1}{48}\ (\frac{2m}{\hbar^2})^2$ to see that:

$$S4^{H.O.} = \frac{1}{24}\{(\frac{2m}{\hbar^2})\frac{2k^2}{7}\ (\tau - \frac{1}{4} \frac{\hbar^2}{2m}\ \nabla^2\rho) - \frac{3}{35}\ k^4\rho + \frac{k^4}{105\pi^2}\ (\frac{2m}{\hbar^2})^{1/2}\ (\frac{2}{3}\ \frac{\nabla^2 V}{\sqrt{\lambda-V}}$$

$$+ \frac{9}{4}\ (\frac{(\nabla V)^2}{(\lambda-V)^{3/2}}))\}\, \theta(\lambda-V) . \qquad (16)$$

If we compare (16) with (12) we see that they are identical.

We may do a similar calculation for the S^6 coefficient. We neglect the factor $-\frac{1}{576}\left(\frac{2m}{\hbar^2}\right)^3$ and write:

$$S6^{H.O.} = \int_Q^\infty \int_{r'}^\infty \tau(r'') - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(r''))\frac{dV}{dr''}\,dr''\,\frac{dV}{dr'}\,dr' \qquad (17)$$

If we use (9) in the integrand, the first integral is simply (15). We then note that:

$$-\frac{1}{6\frac{dV}{dr}}\frac{d}{dr}\{(\lambda-V)^{3/2}(\nabla V)^2\} = \{\frac{1}{4}\sqrt{\lambda-V}\left(\frac{dV}{dr}\right)^2 - \frac{1}{3}(\lambda-V)^{3/2}\frac{d^2V}{dr^2}\}.$$

This may be used to integrate (15) with the result that:

$$S6^{H.O.} = \left(\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{4}{315\pi^2}(\lambda-V)^{9/2} + \left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{1}{24\pi^2}(\lambda-V)^{3/2}(\nabla V)^2\right)\theta(\lambda-V). \qquad (18)$$

Using (6) through (9) we may re-arrange (8) in the following from, including the factor $-\frac{1}{576}\left(\frac{2m}{\hbar^2}\right)^3$:

$$S6^{H.O.} = -\frac{1}{432}\{\left(\frac{2m}{\hbar^2}\right)\frac{1}{7}k^4\left(\tau - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2 p\right) - \frac{2}{35}k^6\rho + \frac{k^6}{105\pi^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\left(\frac{\nabla^2 V}{\sqrt{\lambda-V}} + \frac{11}{4}\frac{(\nabla V)^2}{(\lambda-V)^{3/2}}\right\}\theta(\lambda-V)\,. \qquad (19)$$

Upon comparing (19) with (12), we see that the S^6 coefficients are identical. Therefore we see that if we make a semi-classical approximation on the integrand in (1.53), and further assume $\nabla^2 V = 3V'' = \text{constant}$; then at least up to the S^6 coefficient (1.53) reduces to (12).

iii) The Connection with the Approach of Negele and Vautherin

The form of (5) and (1) are similar. Using the recurrence[4] relation between Bessel functions, we may rewrite (5) as:

$$\overline{\rho^J(\underset{\sim}{Q},\underset{\sim}{S})} = \{\rho(\underset{\sim}{Q})\hat{j}_1(kS) + \frac{1}{6}\,[(\frac{1}{4}\,\frac{\hbar^2}{2m}\,\nabla^2\rho - \tau)\,\frac{2m}{\hbar^2} + \frac{3}{5}\,k^2\rho]\hat{j}_3(kS)S^2$$

$$+ \frac{1}{126}\,[\frac{k^4}{20\pi^2}\,(\frac{2m}{\hbar^2})^{1/2}(\frac{9}{4}\,\frac{(\nabla V)^2}{(\lambda-V)^{3/2}} + \frac{2}{3}\,\frac{\nabla^2 V}{(\lambda-V)})\hat{j}_3(kS) +$$

$$+ \frac{k^2}{3}\,(\frac{2m}{\hbar^2}\,(\tau - \frac{1}{4}\,\frac{\hbar^2}{2m}\,\nabla^2\rho) - \frac{3}{5}\,k^2\rho)\hat{j}_4(kS)]S^4$$

$$- \frac{1}{45360\pi^2}\,k^6\,(\frac{2m}{\hbar^2})^{1/2}[\frac{1}{2}\,\frac{(\nabla V)^2}{(\lambda-V)^{3/2}} + \frac{1}{3}\,\frac{\nabla^2 V}{(\lambda-V)^{1/2}}]\hat{j}_4(kS)S^6\}\theta(\lambda-V). \quad (20)$$

Note that the first line is identical in form to (5) and hence, if we neglect all terms which go to zero faster than S^2, we have:

$$\overline{\rho^J(\underset{\sim}{Q},\underset{\sim}{S})} = \{\rho(\underset{\sim}{Q})\hat{j}_1(kS) + \frac{1}{6}[(\frac{1}{4}\nabla^2\rho - \tau)\,\frac{2m}{\hbar^2} + \frac{3}{5}\,k^2\rho]\hat{j}_3(kS)S^2\{\theta(\lambda-V). \quad (21)$$

We see that (21) has the same form as (5) but the following differences occur: ρ and τ are given by their semi-classical expressions, and k does not equal k_F, since ρ is not the Thomas Fermi ρ, but the extended Thomas Fermi ρ. Hence $k \neq (3\pi^2\rho)^{1/3}$. Also, since we are using semi-classical quantities, (21) is valid only to the turning point. If we accept (21) as the proper way to write $\rho^{N.V.}(\underset{\sim}{Q},\underset{\sim}{S})$ in the semi-classical approximation, we may then use the results of the previous section.

If we expand (20) in a series of S^2, we will have the same result as (12). Therefore, the expansion of (20) is equivalent to our harmonic approximation, as shown in section ii). We then subtract off the contributions from the terms neglected in going from (20) to (21) to find:

$$S4^{H.O.} = \left(\frac{1}{108}\, k^2 \left(\frac{2m}{\hbar^2}\right)\left(\tau - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho\right) - \frac{1}{504}\, k^4\rho\right)\theta(\lambda-V) \quad (22)$$

and

$$S6^{H.O.} = -\frac{1}{432}\left(\frac{1}{11}\, k^4\, \frac{2m}{\hbar^2}\left(\tau - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho\right) + \frac{2}{77}\, k^6\rho\right)\theta(\lambda-V) \quad (23)$$

which are the corresponding terms to (10).

Hence, we have shown that within the semi-classical approximation, if certain terms are neglected, (1.53) may be reduced to the Negele-Vautherin form, at least to the sixth order coefficient.

iv) <u>The Connection with the Campi-Bouyssy Approach</u>

It was not possible to reproduce the Campi-Bouyssy expression when one uses expressions (6) through (9). However, if we use the Thomas-Fermi expressions for the relevant quantities, which are simply the first terms in (6) through (9), we can derive (3) from (1.53).

The general term in our harmonic approximation is:

$$SN^{H.O.} = \frac{2}{3.4^n n!} \left(\frac{2m}{\hbar^2}\right)^n \int_r^\infty \cdots \int_{r_{n-2}}^\infty \left(\tau(r_{n-1}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(r_{n-1})\right) \frac{dV}{dr_{n-1}}\, dr_{n-1} \cdots \frac{dV}{dr_1}\, dr_1 \,. \qquad (24)$$

In the Thomas-Fermi approximation we have:

$$\tau - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho = \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{1}{5\pi^2} (\lambda-V)^{5/2} \,. \qquad (25)$$

If we integrate (25) (n-1) times with respect to V, we obtain:

$$\iint \cdots \int (\lambda-V)^{5/2} dV_{n-1} \cdots dV_1 = \frac{3.2^{n-1}}{(2n+3)!!} (\lambda-V)^{2n+3/2} \qquad (26)$$

and therefore our general term becomes:

$$SN^{H.O.} = \frac{1}{2^n n!(2n+3)!!} \left(\frac{2m}{\hbar^2}\right)^{(2n+3)/2} \frac{(\lambda-V)^{(2n+3)/2}}{2} \,. \qquad (27)$$

We note that $\rho^{T.F.}$ is:

$$\rho^{T.F.} = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} (\lambda-V)^{3/2} \qquad (28)$$

and therefore we may write (27) as:

$$SN^{H.O.} = 6 \cdot \frac{n+1}{(2n+3)!} \left(\frac{5}{3}\right)^n \left(\frac{2m}{\hbar^2}\right)^n \frac{\left(\tau - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho\right)^n}{\rho^{n-1}} \tag{29}$$

where we have rewritten $(2n+3)!!$ as $(2n+3)!/((n+1)!2^{n+1})$.

We note that the S'th term of $\hat{j}_i(x)$ is:

$$6 \cdot \frac{S+1}{(2S+3)!} x^{2S}, \tag{30}$$

and then substituting this for the n'th order Campi-Bouyssy term given by (3), we have:

$$SN^{C.B.} = \rho \cdot 6 \cdot \frac{n+1}{(2n+1)!} \left(\frac{2m}{\hbar^2}\right)^n \left(\frac{5}{3}\right)^n \frac{\left(\tau - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho\right)^n}{\rho^n} \tag{31}$$

which is identical to (29).

Hence we have shown that under the Thomas-Fermi approximation (1.53) can be reduced to the Campi-Bouyssy form to all orders in S^2.

CHAPTER 3

NUMERICAL RESULTS

i) One Dimension

It is interesting to see how good an approximation (1.39), the HOA, is, compared to the exact result in one dimention (1.15). We also compare the one dimensional forms of the Negele-Vautherin (NVA) and Campi-Bouyssy (CBA) approximation. Since they all agree up to the s^2 coefficient we shall limit discussion in this section to the s^4 coefficient.

The NVA in one dimension is derived by Sprung, et al (1975) and is given in equation (1).

$$\rho^{NV}(q,s) = \rho(q)\hat{j}_0(k_F s) + \frac{s^2}{2}\left(\frac{2m}{\hbar^2}\left(\frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2\rho(q)}{dq^2} - \tau(q) + \frac{1}{3}k_F{}^2\rho(q)\right)\right)\hat{j}_2(k_F s) \tag{1}$$

where $k_F = \pi\rho(q)$.

It is also easy to write down the CBA in one dimension

$$\rho^{CB}(q,s) = \rho(q)\hat{j}_0(\hat{k}s) \quad . \tag{2}$$

In this case the effective momentum $\hat{k}$ is given by:

$$\hat{k} = \left(\frac{3}{\rho(q)}\frac{2m}{\hbar^2}\left(\tau(q) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2\rho(q)}{dq^2}\right)\right)^{1/2} \tag{3}$$

We expand the one dimensional forms (1), (2), (1.39) and (1.15) in a Taylor series and denote the s^4 coefficients as follows:

$$\text{i)}\quad S4^{EX} = \frac{1}{192} \sum_{i=1}^{N} g_i \{ \psi_i(q) \frac{d^4\psi_i(q)}{dq^4} - 4 \frac{d\psi_i(q)}{dq} \frac{d^3\psi_i(q)}{dq^3} + 3 (\frac{d^2\psi_i(q)}{dq^2})^2 \}$$

$$\text{ii)}\quad S4^{HO} = \frac{1}{16} (\frac{2m}{\hbar^2})^2 \int_q^\infty (\tau(r) - \frac{1}{4} \frac{\hbar^2}{2m} \frac{d^2\rho(r)}{dr}) \frac{dV}{dr} dr$$

$$\text{iii)}\quad S4^{CB} = \frac{3}{40\rho(q)} (\frac{2m}{\hbar^2})^2 (\tau(q) - \frac{1}{4} \frac{\hbar^2}{2m} \frac{d^2\rho(q)}{dq^2})^2$$

$$\text{iv)}\quad S4^{NV} = \frac{\pi^2}{28} \rho^2(q) \frac{2m}{\hbar^2} (\tau(q) - \frac{1}{4} \frac{\hbar^2}{2m} \frac{d^2\rho(q)}{dq^2}) - \frac{\pi^4}{280} \rho^5(q) . \qquad (4)$$

It is not possible to analyze equations (4) in general, so a model potential was chosen. The Eckart potential, given in equation (5) was used in one dimensional calculations.

$$V(q) = - \frac{\hbar^2}{2m} \alpha^2 \gamma(\gamma+1) \mathrm{sech}^2(\alpha x) \qquad (5)$$

where α is the effective range parameter and γ is a well depth parameter. The maximum number of bound states is less than or equal to $(\gamma+1)$.

Since there are no one dimensional nuclei, the particular values of α and γ are somewhat arbitrary. We chose to fit them to the values given by Easson, et al (1979) for nuclear matter in one dimension. They assume a binding energy per particle of 5 MeV and a saturation density of 1.44 nucleons per Fermi for the case of 4 nucleons per level. These values are satisfied by fixing the well depth so that $\frac{h^2}{2m}\alpha^2\gamma(\gamma+1) = 30$ Mev with:

$$\alpha = 2.540/A \text{ fm}^{-1} \qquad (6)$$

$$\gamma = \sqrt{1.0+0.896A^2} - 0.5 . \qquad (7)$$

A is the number of particles in the model nucleus.

The eigenfunctions of a Hamiltonian with an Eckart potential are known analytically (Nieto, 1978). The (unnormalized) wavefunctions have the form: $ch^{-\gamma}(\alpha x)$ multiplying a hypergeometric polynomial in $sh(\alpha x)$. These analytic wavefunctions were used in evaluating equations (4).

A summary of the calculations may be found in table I and figures (1) and (2). When there are 4 occupied levels, with 4 particles per level, both $S4^{HO}$ and $S4^{CB}$ are quite accurate, with errors typically less than 5% out to several Fermis. However, as can be seen from figure 1(a) and table IA, when only 2 levels are occupied, the error is around 15% in the interior and the HOA is not even of the correct order of magnitude beyond 4 or 5 Fermis. It was found that as A increased, both $S4^{CB}$ and $S4^{HO}$ improved, both in accuracy, and the region over which they were accurate.

In the case of CBA this is to be expected from the nature of the approximation made in deriving the formula. In

TABLE I

Derivatives of the Eckart Potential

A q	2 levels relative error	$V^{(2)}$	$V^{(3)}$	$V^{(3)}/V^{(2)}$
0.0	.147	1.38	0.00	0.0
1.0	.146	1.09	-2.46	-2.26
2.0	.118	0.11	-4.84	-4.4
3.0	.007	-1.98	-4.93	2.49
4.0	-0.376	-6.06	8.32	-1.40
5.0	-4.80	-13.82	79.88	-5.78
6.0	2.13	-28.49	380.01	-13.0
8.0	1.15	-108.49	5803	-54.0
10.0	1.04	-393.38	77000	-196

B q	4 levels relative error	$V^{(2)}$	$V^{(3)}$	$V^{(3)}/V^{(2)}$
0.0	0.039	1.38	0.00	0.0
1.0	0.039	1.31	-1.22	-0.93
2.0	0.037	1.10	-2.46	-2.24
3.0	0.035	0.71	-3.71	-5.23
4.0	0.033	0.11	-4.83	-43.9
5.0	0.026	-0.75	-5.50	7.33
6.0	0.008	-1.98	-4.93	2.48
7.0	-0.026	-3.69	-1.44	0.39
8.0	-0.084	-6.06	8.32	-1.40
9.0	-0.184	-9.32	31.07	-3.33
10.0	-0.363	-13.82	79.88	-5.78
12.0	-1.75	-28.40	380.0	-13.3
14.0	3.92	-56.20	1534	-27.3

q = centre of mass coordinate

relative error = $(S4^{EX} - S4^{HO})/S4^{EX}$

$V^{(n)}$ are defined in equation (8).

Figure 1

The S^4 coefficients of the density matrix in a one dimensional Eckart potential as a function of the centre of mass coordinate.

Solid line : $S4^{EX}$
Dotted line: S^{HO}
Dashed line: $S4^{CB}$
Dash dot : $S4^{NV}$

where these terms are given by equations (4).

(a) 8 particles in 2 levels [†]

(b) 16 particles in 4 levels.

[†] Note that the kink in figure (a) is an interpolation error.

FIGURE Ia)

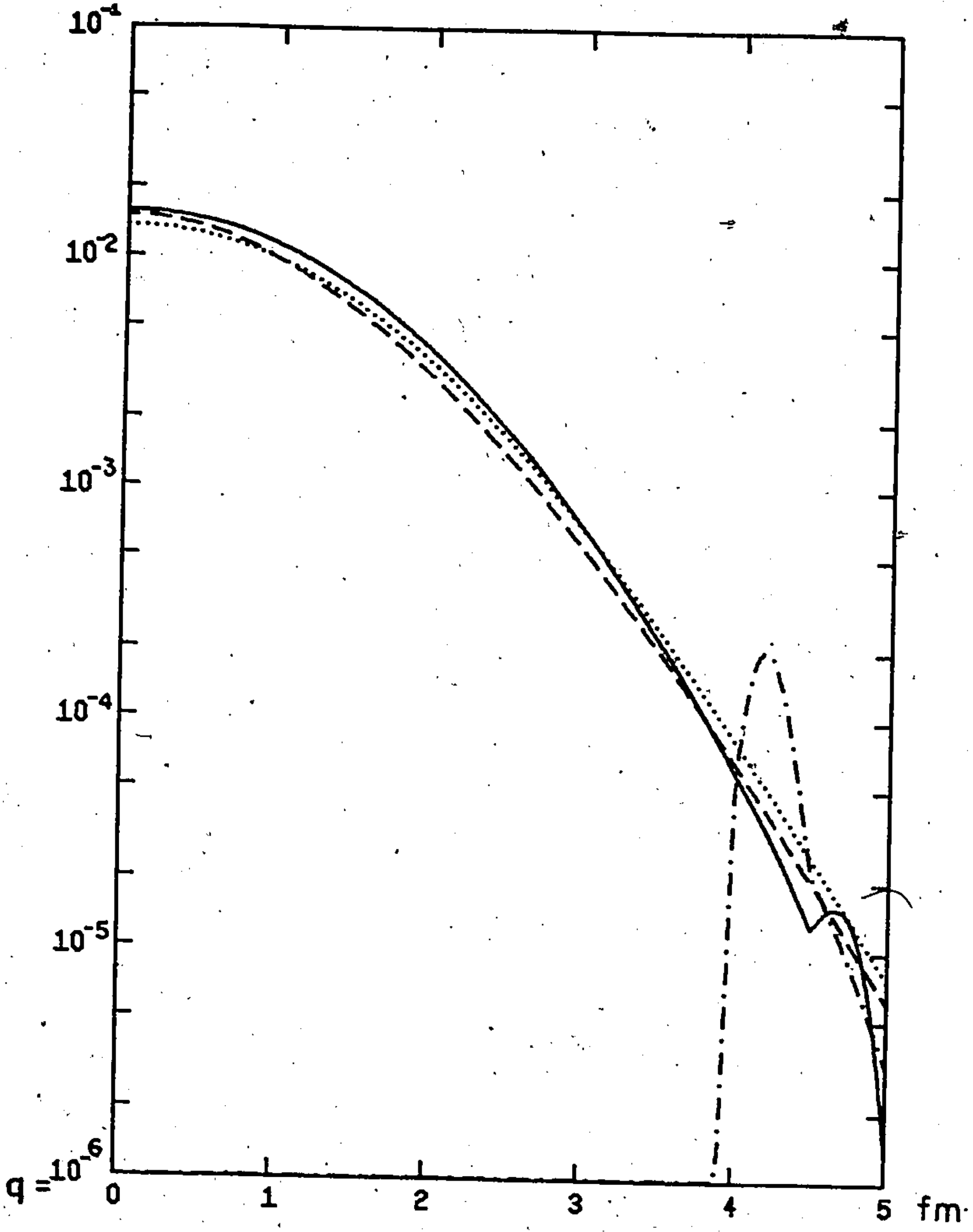


FIGURE 1b)

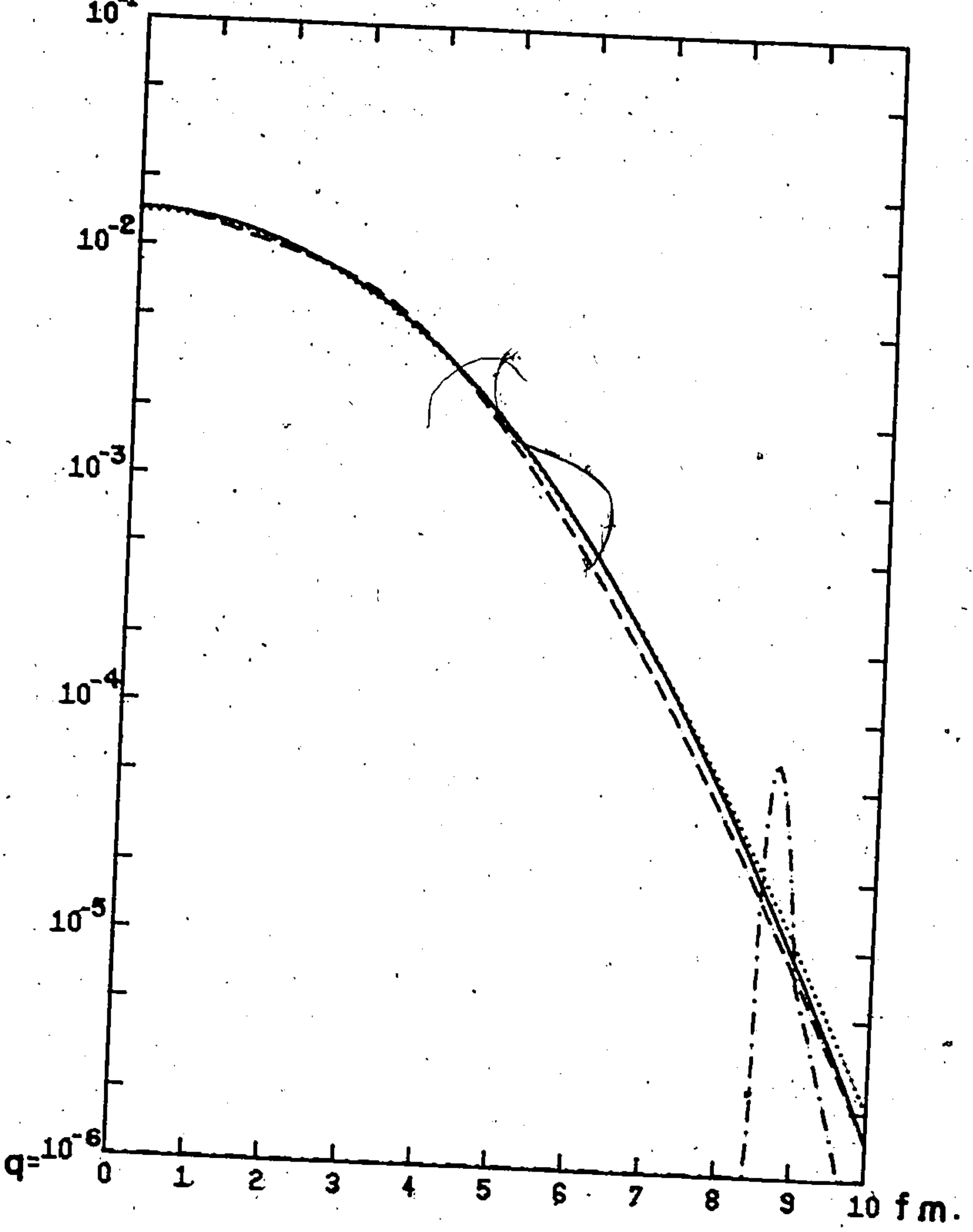


Figure 2

(a) Relative error of the various approximations to the S^4 coefficient of the density matrix for 16 particles in a one dimensional Eckart potential as a function of the centre of mass coordinate.

Solid line : $(S4^{EX}-S4^{HO})/S4^{EX}$

Dashed line : $(S4^{EX}-S4^{CB})/S4^{EX}$

Dotted line : $(S4^{EX}-S4^{NV})/S4^{EX}$

(b) Derivatives of the Eckart potential with 16 particles as a function of the centre of mass coordinate.

Solid line : $V^{(2)}$

Dotted line : $V^{(3)}$

Dashed line : $V^{(4)}$

where $V^{(n)}$ are defined in equation (8).

FIGURE 2a)

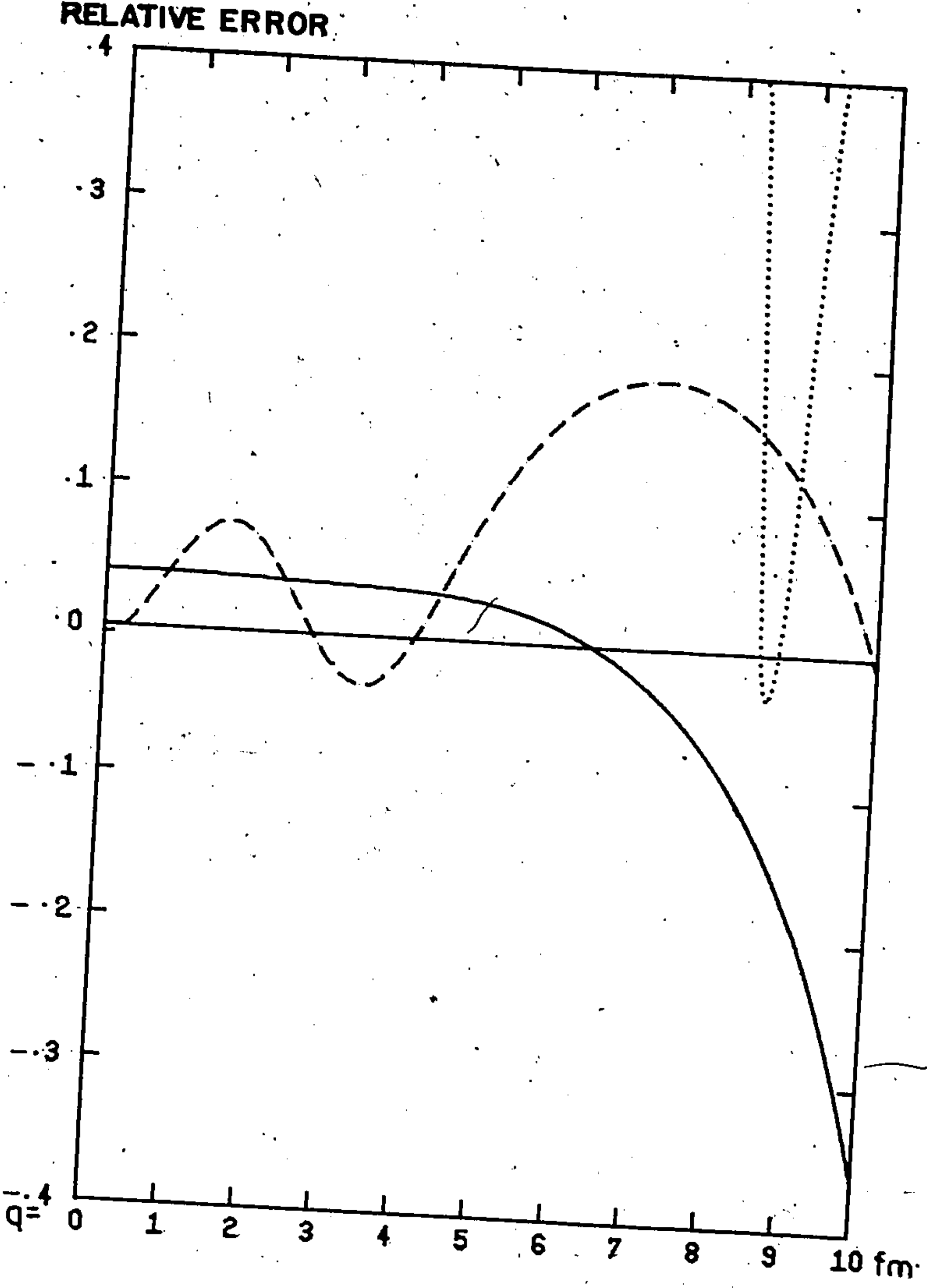
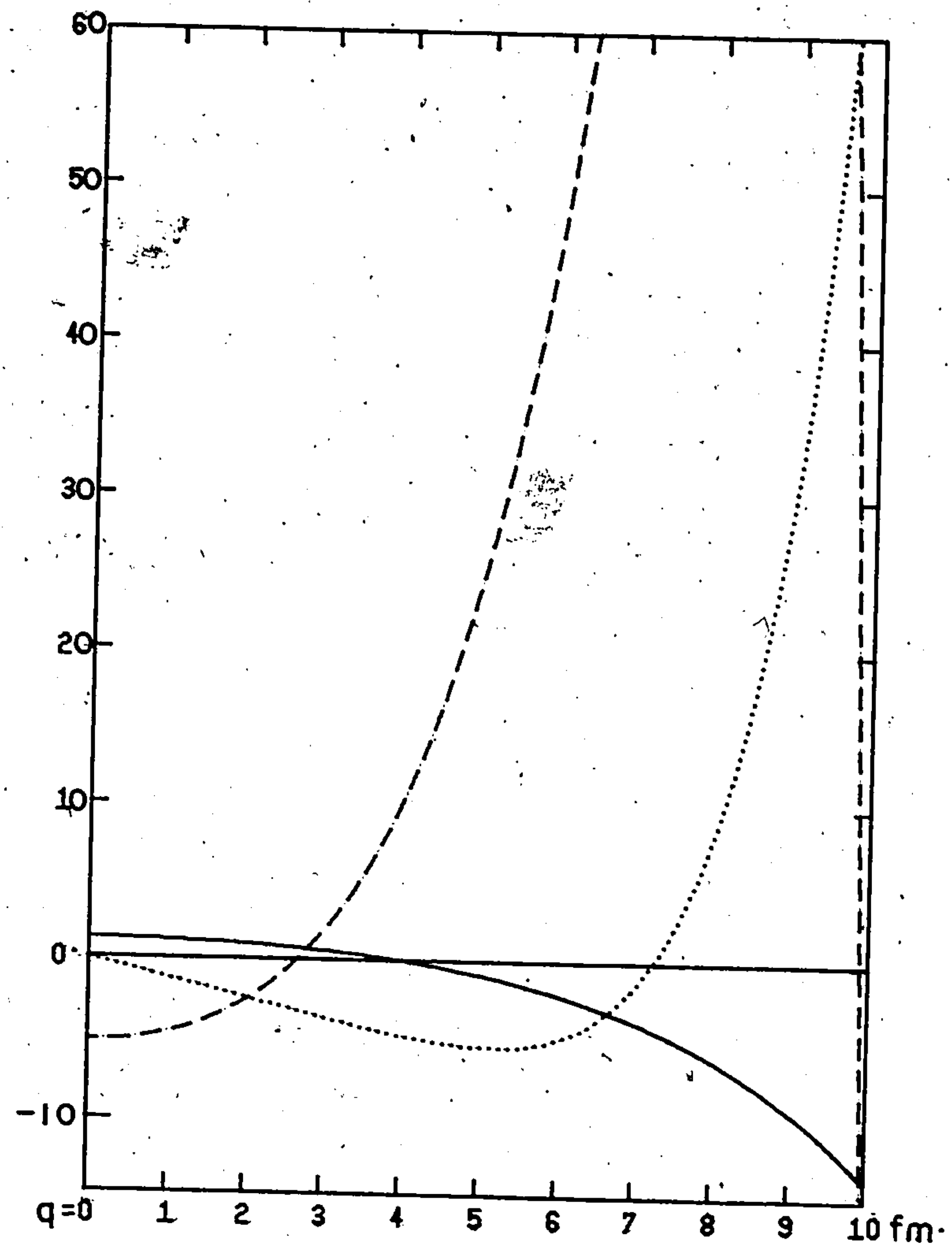


FIGURE 2b)



the case of the HOA, one might expect that this is because the potential well becomes more "flat" in the bottom as A increases, and hence becomes more like a harmonic oscillator potential. In table I, we may note that $V^{(2)}$ (see equation 8)) changes much more slowly for 4 levels, and hence is more nearly a constant as is the case for the harmonic oscillator, when compared with $V^{(2)}$ for 2 levels. This effect is due to the 1/A dependence of α. As A increases, α decreases, and hence V(z) varies more slowly. This is a common feature of smooth one body nuclear potentials (e.g., the Woods Saxon), due to the occurence of saturation. Hence we may expect the HOA to be more accurate for heavy nuclei.

Since the HOA is based on the fact that the second derivative of the potential was constant, and higher derivatives vanish, it is useful to see the correlation between the accuracy of the HOA and the magnitude of the derivatives. We used nondimensionalized derivatives in table I and figure 2b), as given by (8).

$$V^{(n)} = \frac{d^n V}{dq^n} \frac{1}{\alpha^n V^n} \qquad (8)$$

where α, given in (6), defines a length scale.

Table IB and figure 2b) show that when the ratio $V^{(3)}/V^{(2)}$ is less than 10, the HOA gives at least the correct order of magnitude, with one exception, at 4 Fermis. This is due to the fact that $V^{(2)}$ is changing sign here, and hence has a very small magnitude. However, one can see in figure 2b) that both $V^{(2)}$ and $V^{(3)}$ are smooth and not very large at this point.

It is difficult to draw any quantitative conclusions from this, but qualitatively we see that when V varies slowly as a function of x, the HOA does give a good approximation to the fourth order coefficient.

Finally, we may comment on the very poor agreement between $S4^{NV}$ and $S4^{EX}$. The case where $\gamma=1$ and only one level is occupied may be done easily and hence it is instructive to look at this case.

$$\rho(q,s) = \frac{\alpha}{2}\,\frac{1}{ch(2\alpha q)+ch(\alpha s)} \text{ (for one particle per level).} \qquad (9)$$

We may expand (9), and note that:

$$\frac{2m}{\hbar^2}\left(\tau(q) - \frac{1}{4}\,\frac{\hbar^2}{2m}\,\frac{d^2\rho(q)}{dq^2}\right) = \alpha^2\rho(q)$$

to write

i) $S4^{EX} = \dfrac{\alpha^2\rho^3}{4} - \dfrac{\alpha^3\rho^2}{24}$

ii) $S4^{HO} = \dfrac{\alpha^2\rho^3}{12}$

iii) $S4^{CB} = \dfrac{3\alpha^2\rho^3}{40}$

iv) $SN^{NV} = \pi^2\alpha\rho^4/28 - \pi^4\rho^5/280.$ (10)

For the values of $\rho(q)$ used, it was found that 10 iv) overestimates the exact s^4 coefficient by about two orders of magnitude in the interior, and is of the wrong sign. It also falls off much more quickly than 10 i) in the tail. This is understandable, since 10 iv) has a much stronger dependence on ρ than 10 i), 10 ii) or 10 iii); all of which agree to within 20% or better for several Fermis and for different numbers of levels. Hence it appears that the Negele-Vautherin form is not suitable for one dimensional calculations, at least for a model potential similar to the Eckart potential.

Also, since the Eckart potential is similar to a harmonic oscillator potential, at least in the interior, the above analysis sheds light on some speculations of Sprung, et al (1975A). They analyzed the Negele-Vautherin expansion using the Bloch density matrix for the harmonic oscillator in one dimension (see equation 1.32). Our analysis shows that for the sharp Fermi surface case this expansion is not accurate. Out to about one Fermi (with four particles occupying the ground state), the fourth order coefficient is actually larger than the leading term.

Hence we may conclude that the HOA and the CBA can be accurate for one dimensional systems if they are large enough. The NVA does not appear to be very good at all in reproducing the one dimensional density matrix (at least to fourth order).

ii) Three Dimensions

In this section we have checked the various approximations in three dimensions, expanded in a Taylor series to S^4. The exact angle averaged density matrix, $\overline{\rho(Q,S)}$, up to S^4 is given by (B28). The HOA in three dimensions is given by (1.53). We also truncated (2.10), the CBA, and (2.11), the NVA, to fourth order. In this section when we refer to the above expressions, we shall mean the expansions truncated to fourth order in $\underset{\sim}{S}$. As mentioned above, the three approximations are exact up to S^2 and differ only in the S^4 and higher coefficients. We reproduce the S^4 coefficients below.

$$S4^{EX} = \frac{1}{960}\Big\{\frac{2m}{\hbar^2}\big(\rho(\underset{\sim}{Q})\nabla^2 V(Q) - \nabla\rho(\underset{\sim}{Q})\cdot\nabla V(Q)\big)$$

$$+ \left(\frac{2m}{\hbar^2}\right)^2 \sum_{n,\ell}\Big(2(V(Q)-\varepsilon_{n,\ell})^2 R^2_{n,\ell}(\underset{\sim}{Q})\,\frac{2\ell+1}{\pi} - 4(V(Q)-\varepsilon_{n,\ell})\,\tau_{n,\ell}(\underset{\sim}{Q})\Big)$$

$$+ 2\sum_{n,\ell,m}\nabla\nabla\psi^*_{n,\ell,m}(\underset{\sim}{Q}):\nabla\nabla\psi_{n,\ell,m}(\underset{\sim}{Q})\Big\} \qquad (11(i))$$

$$S4^{HO} = \frac{1}{48}\left(\frac{2m}{\hbar^2}\right)^2 \int_Q^\infty \left(\tau(\underset{\sim}{R}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{R})\right)\frac{dV}{dR}\,dR \qquad (11(ii))$$

$$S4^{CB} = \frac{5}{504}\left(\frac{2m}{\hbar^2}\right)^2\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right)^2\Big/\rho(\underset{\sim}{Q}) \qquad (11(iii))$$

$$S4^{NV} = \frac{k_F^2}{108}\,\frac{2m}{\hbar^2}\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right) - \frac{k_F^4}{504}\,\rho(\underset{\sim}{Q}) \qquad (11(iv)$$

$\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}$ and the three approximations were tested on two potentials; the harmonic oscillator with $\hbar\omega = 41/A^{1/3}$ MeV and the Woods Saxon with a well depth of 44 MeV and an effective range parameter of 1.27 $A^{1/3}$ fm. The scaling in the exponential, a_0, was chosen to be 0.67 fm. The harmonic oscillator potential was chosen as a test case, since analytic expressions could be calculated, and since the HOA would be exact in this case. The Woods Saxon was chosen as a more "realistic" potential for the nuclear case, as we are interested in checking this approximation for nuclei. All calculations assumed equal numbers of protons and neutrons, and ignored the coulomb energy and spin orbit splitting.

For both potentials we calculated $\rho(\underset{\sim}{Q},\underset{\sim}{S})$ and the three approximations, and then normalized the result to the local density $\rho(\underset{\sim}{Q})$. This enabled us to compare the accuracy of the approximations as a function of $\underset{\sim}{S}$ for various values of $\underset{\sim}{Q}$ measured from the centre of the nucleus. We show the results for ^{16}O and ^{40}Ca; both considered in a Woods Saxon potential; in figures 3) and 5) respectively.

Equations (11) were also calculated separately and analyzed as a function of the centre of mass coordinate $\underset{\sim}{Q}$. The results for ^{16}O and ^{40}Ca are shown in figures 4) and 6). Although these figures show how well each approximation reproduces the shape of $S4^{EX}$, it is difficult to establish how accurate the approximation was. Therefore we integrated $S4^{EX}$ and the approximations as a function of $\underset{\sim}{Q}$. These appear in

Figure 3

The angle averaged density matrix of ^{16}O in a Woods Saxon potential

Solid line : $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}/\rho(\underset{\sim}{Q})$
Dotted line : $\overline{\rho_2(\underset{\sim}{Q},\underset{\sim}{S})}/\rho(\underset{\sim}{Q})$
Dashed line : $HOA/\rho(\underset{\sim}{Q})$
Dashed single dot : $CBA/\rho(\underset{\sim}{Q})$
Dashed double dot : $NVA/\rho(\underset{\sim}{Q})$

where $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}$ is given up to fourth order in $\underset{\sim}{S}$ by (B28)
$\overline{\rho_2(\underset{\sim}{Q},\underset{\sim}{S})}$ is (B28) truncated at S^2
HOA is given up to fourth order in (1.53)
CBA is (2.10) truncated to fourth order
NVA is (2.11) truncated to fourth order

FIGURE 3

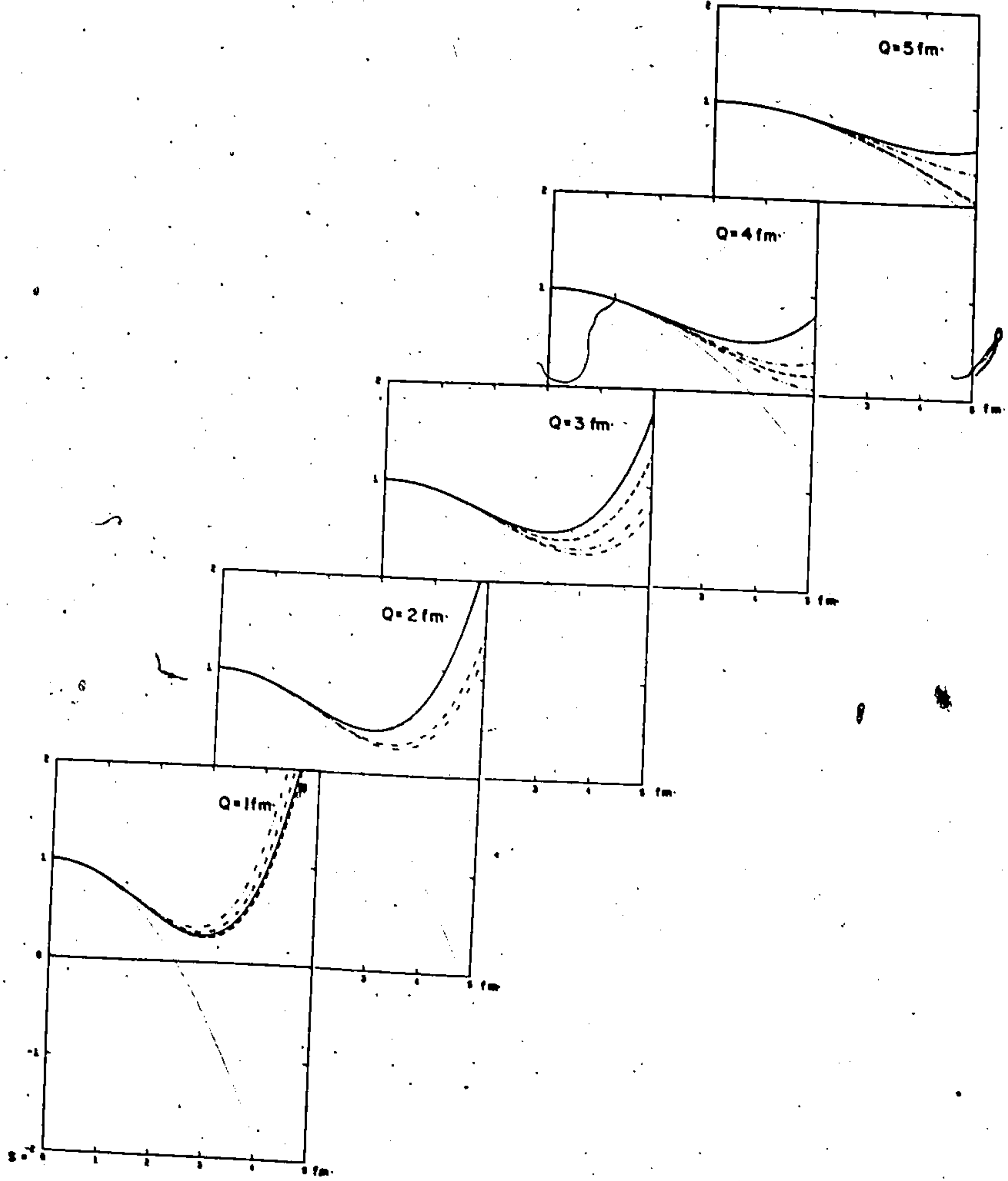


Figure 4

The S^4 coefficients of the angle averaged density matrix for ^{16}O in a Woods Saxon potential as a function of the centre of mass coordinate.

Solid line : $S4^{EX}$
Dotted line : $S4^{HO}$
Dashed line : $S4^{CB}$
Dashed dot : $S4^{NV}$

Figure (4a) : to 5 fm.
Figure (4b) : to 10 fm.

FIGURE 4 a)

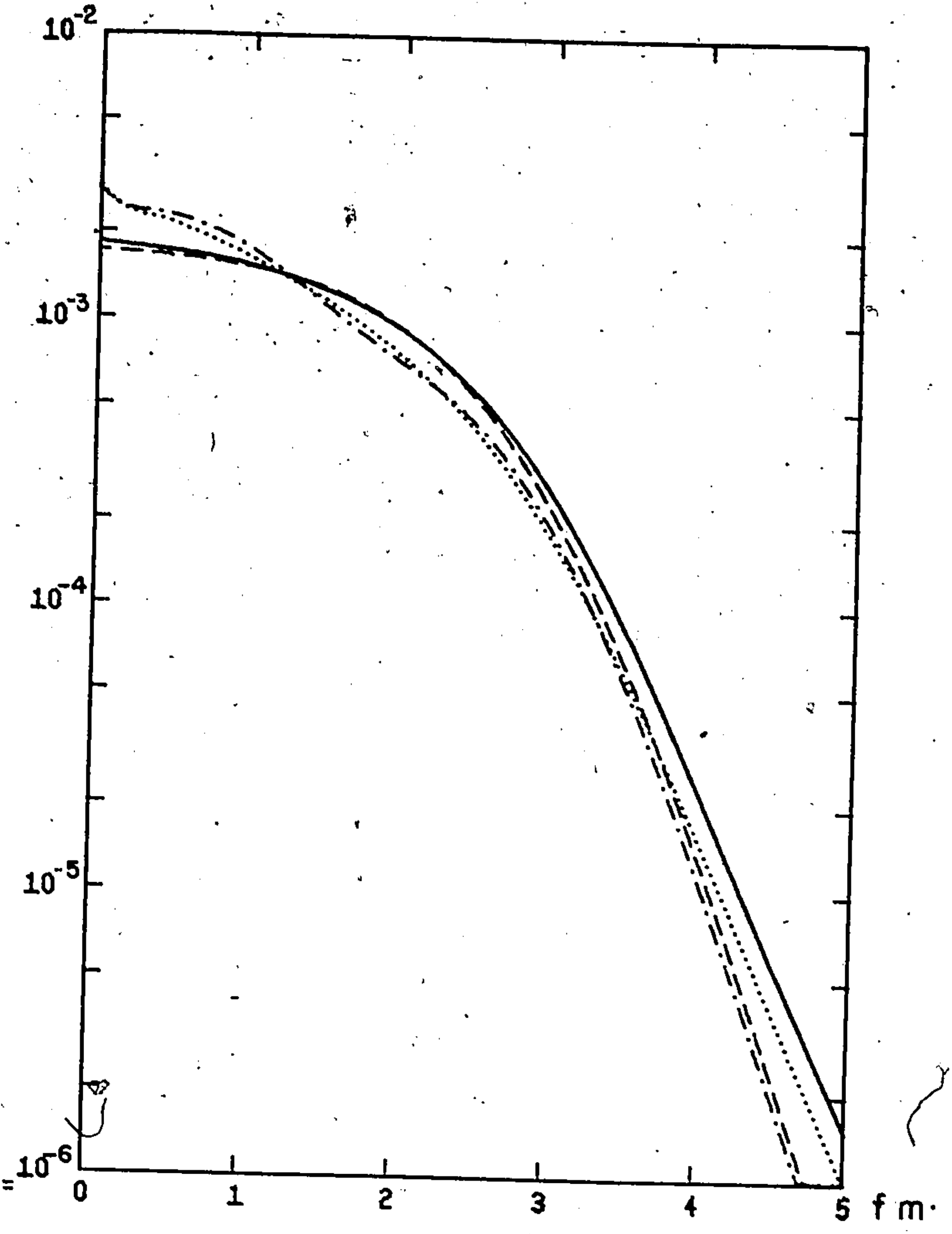


FIGURE 4 b)

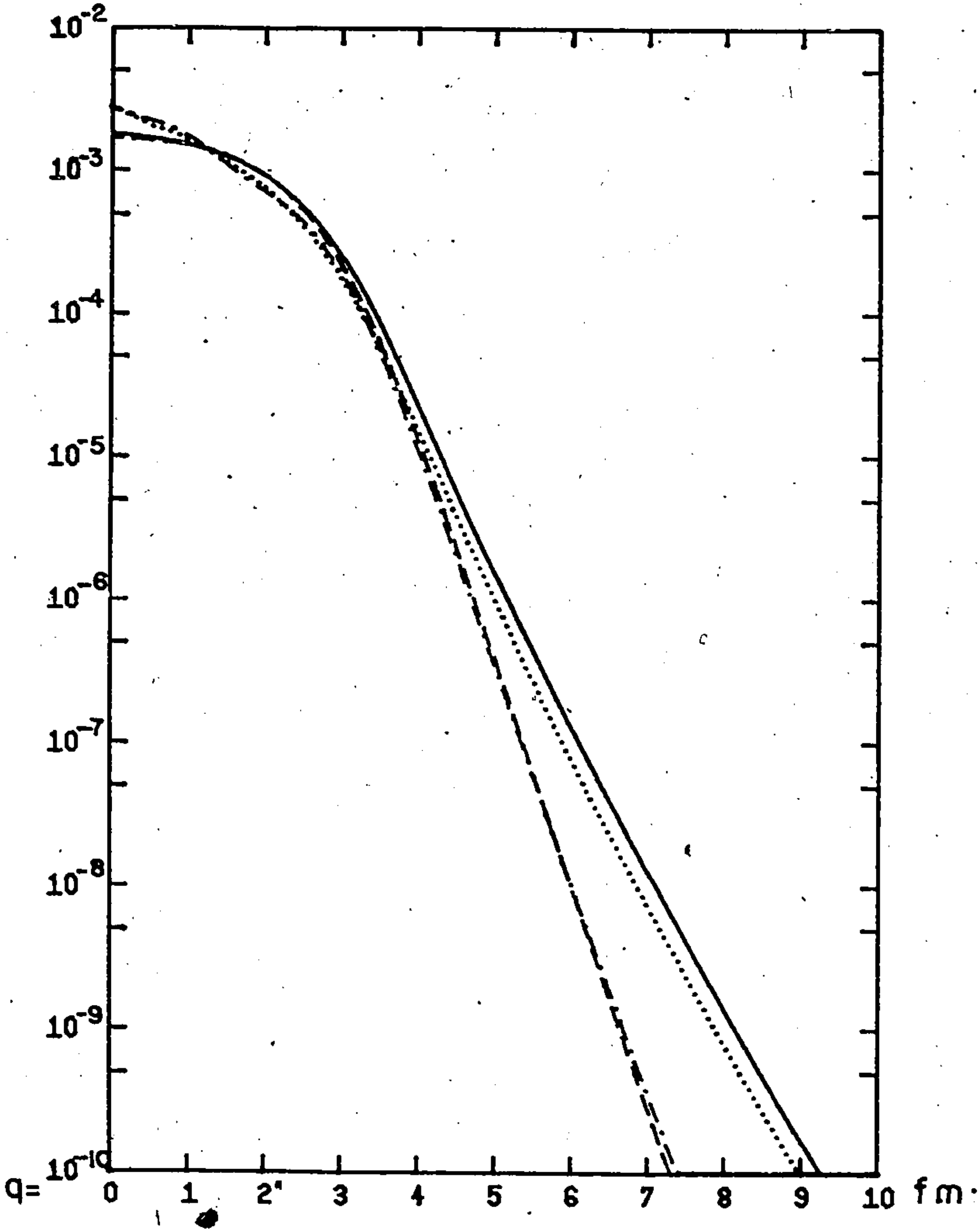


Figure 5

The angle averaged density matrix for ^{40}Ca in a Woods Saxon potential

Solid line : $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}/\rho(\underset{\sim}{Q})$

Dotted line : $\overline{\rho_2(\underset{\sim}{Q},\underset{\sim}{S})}/\rho(\underset{\sim}{Q})$

Dashed line : $HOA/\rho(\underset{\sim}{Q})$

Dashed single dot : $CBA/\rho(\underset{\sim}{Q})$

Dashed double dot : $NVA/\rho(\underset{\sim}{Q})$.

FIGURE 5

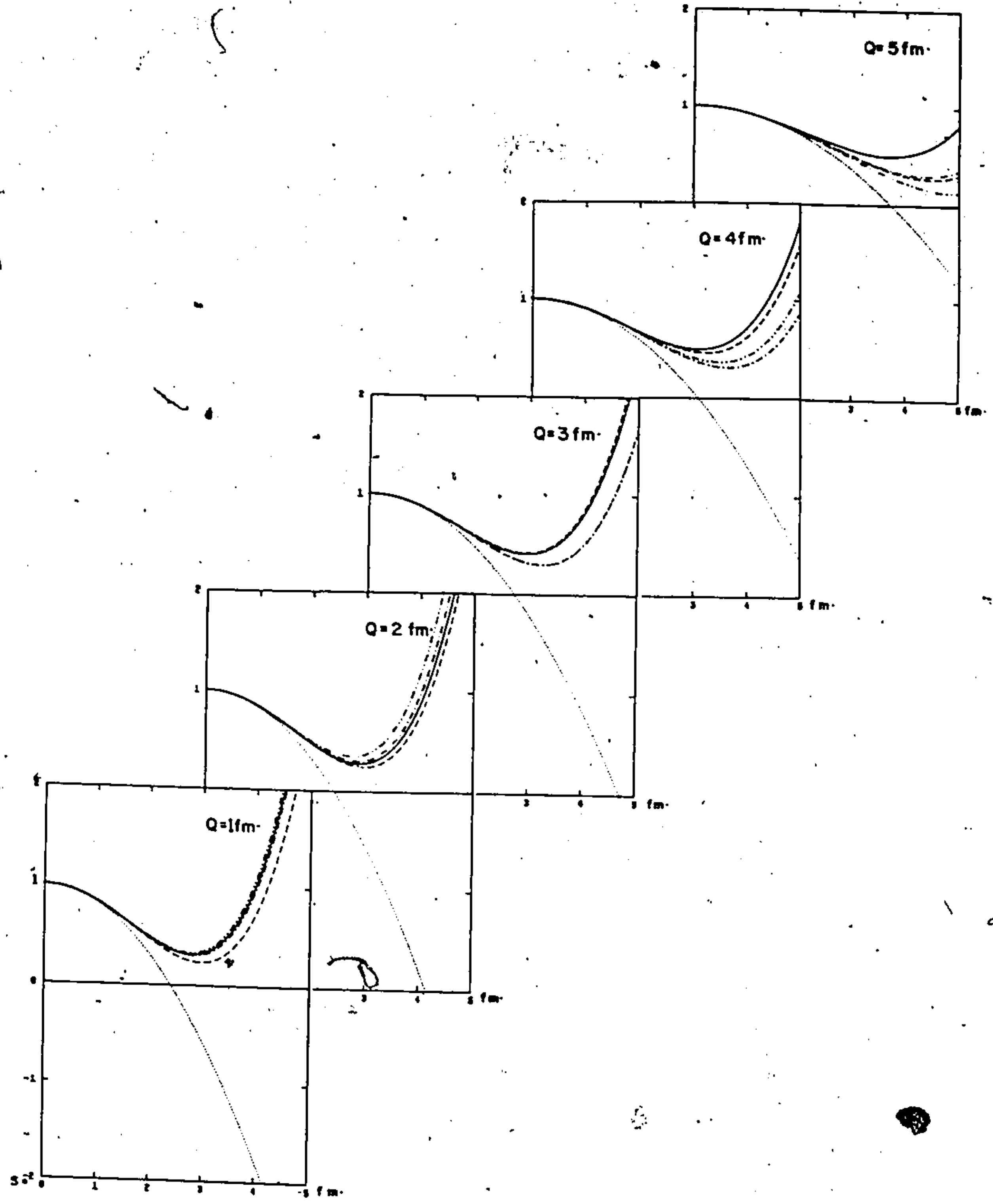


Figure 6

The S^4 coefficients of the angle averaged density matrix for ^{40}Ca in a Woods Saxon potential as a function of the centre of mass coordinate.

Solid line : $S4^{EX}$
Dotted line : $S4^{HO}$
Dashed line : $S4^{CB}$
Dash dot : $S4^{NB}$

Figure 6a : to 5 fm.
Figure 6b : to 10 fm.

FIGURE 6 a)

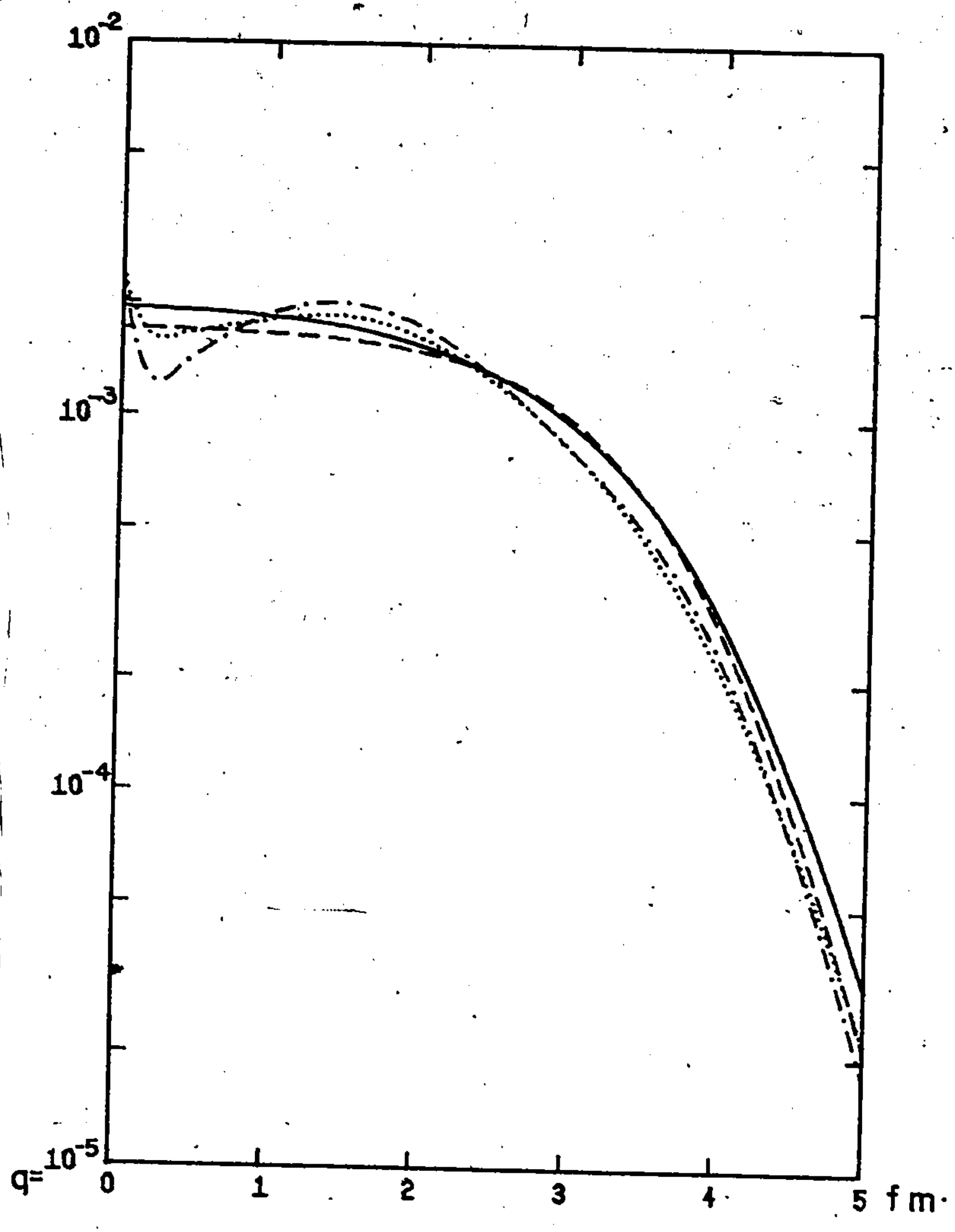


FIGURE 6b)

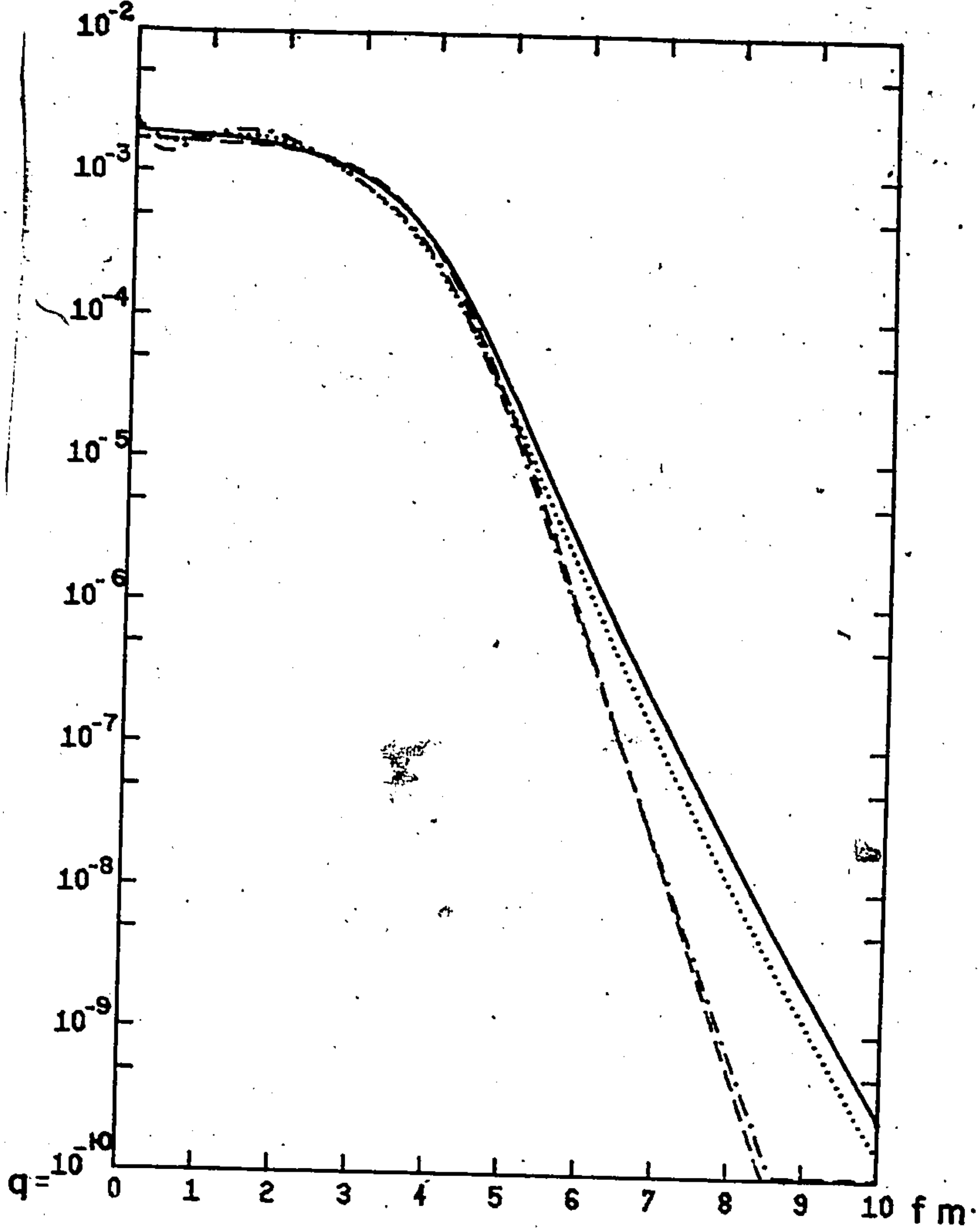


Table II, for several different nuclei, and both potentials.

All these results are similar to the one dimensional results. As A increases, the accuracy of $S4^{HO}$ improves and the region over which it is accurate increases (for the Woods Saxon, since it is already exact for the harmonic oscillator potential). It appears that $S4^{HO}$ is accurate to about 0.2 to 0.5 fm. past the r.m.s. radius of the nucleus.

In the extreme surface region, the HOA begins to underestimate $\rho(\underset{\sim}{Q},\underset{\sim}{S})$ by a large amount. This is probably related to the fact that this form is exact for harmonic oscillator wavefunctions which are gaussians asymptotically. However, realistic wavefunctions in a finite potential well have wavefunctions which are exponentials asymptotically. Therefore, a large distance from the centre of the nucleus one might expect this approximation to be too small. However, as can be seen in table II, the integral of $S4^{HO}$ is more accurate than for either of the other approximations. Therefore, it appears that this underestimate in the tail does not have a large effect in the overall result.

As mentioned in chapter 2, the CBA expression is the most accurate approximation in the tail. This is confirmed by our study as can be seen from figures 4 b) and 6 b), where we see that $S4^{CB}$ underestimates $S4^{EX}$ by about 30% in the tail but follows the correct trend. The reason for $S4^{HO}$ underestimating in the tail has been mentioned above.

Table II. Global relations comparing the 0'th, 2'nd and 4'th order terms of the angle averaged density matrix

Potential	$A = \int \rho(\underset{\sim}{Q}) d^3Q$	$\frac{1}{6} \frac{2m}{h^2} T$	$\int S4^{EX} d^3Q$	$\int S4^{HO} d^3Q$	$\int S4^{CB} d^3Q$	$\int S4^{NV} d^3Q$
HO	4.000	0.6223	.04842	.04842	.03459(-.285)	.02595(-.465)
WS	4.000	0.3663	.01898	.01578(-.168)	.01329(-.300)	.01066(-.438)
HO	16.000	2.3517	.1537	.1537	.1287 (-1.53)	.1245 (-.190)
WS	16.000	1.840	.09922	.09293(-.063)	.08102(-.183)	.08091(-.184)
HO	40.000	5.788	.3547	.3547	.3181 (-.103)	.3257 (-.082)
WS	40.000	5.133	.2832	.2719 (-.040)	.2496 (-.119)	.2580 (.089)
HO	140.000	19.978	1.1721*	1.1721	1.1122 (-.051)	1.1723 (+.0002)
WS	140.000	19.458	†	1.0450	1.0376	1.0817

---

[*] This value was not calculated by 11 i) but was assumed to be equal to 11 ii) since the HOA is exact for the harmonic oscillator

[†] No value for this was calculated since T4 (given by B.22)) was not calculated for $\ell > 2$.

The values in brackets are the relative errors with respect to the exact result in column 3.

[T] is the total integrated kinetic energy density.

The first three columns give an idea of the rate of convergence of $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}$.

The expressions for $S4^{CB}$ and $S4^{NV}$ are given below:

$$S4^{CB} = \frac{1}{280}\,\hat{k}^4 \tag{12(i)}$$

$$S4^{NV} = \frac{1}{108}\,\frac{2m}{\hbar^2}\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\,\frac{\hbar^2}{2m}\,\nabla^2\rho(\underset{\sim}{Q})\right)k_F{}^2 - \frac{1}{504}\,k_F{}^4\rho(\underset{\sim}{Q}) \tag{12(ii)}$$

where k_F and $\hat{k}$ are defined in chapter 2. As can be seen from table III, $\hat{k}$ cuts off much more slowly than k_F past the 1/2 density radius, and hence (12(i)) is likely to be much larger there. This has been shown to be true also for the harmonic oscillator potential by Campi and Bouyssy (1978A).

One unexpected point of interest came out in this analysis. If one looks at figure 7) we can see that $|\nabla V|$ and $\nabla^2 V$ are more smooth for ^{40}Ca than for ^{16}O, particularly in the interior of the nucleus. Yet out to about 2 fm. $S4^{HO}$ is more accurate for ^{16}O than for ^{40}Ca, although ^{40}Ca is more accurate overall. This indicates that the smoothness of the derivatives is not of sufficient criterion for deciding on the applicability of the HOA.

We may also note that $S4^{HO}$ reproduces the shape of $S4^{EX}$ more accurately than $S4^{CB}$ or $S4^{NV}$. Therefore, when integrals such as exchange integrals are used, the HOA may given even better results than indicated by table II.

As a final point, it should be mentioned that the HOA was derived only for the ground state of a system, since we

Table III. Fermi Momentum and the C.B. Modified Momentum

A ^{16}O in a Woods Saxon potential

Q	k_F	$\hat{k}$
1.0	1.65	1.32
2.0	1.56	1.13
3.0	1.12	1.01
4.0	.643	.833
5.0	.338	.679
6.0	.177	.583
7.0	.0938	.521
8.0	.0506	.476
9.0	.0277	.441
10.0	.0153	.412

B ^{48}Ca in a Woods Saxon potential

Q	k_F	$\hat{k}$
1.0	1.71	1.32
2.0	1.65	1.32
3.0	1.56	1.16
4.0	1.18	1.03
5.0	.704	.852
6.0	.378	.689
7.0	.200	.584
8.0	.108	.515
9.0	.0590	.466
10.0	.0329	.428

Figure 7

The Woods Saxon potential and its derivatives for ^{16}O and ^{40}Ca

Solid line : Woods Saxon potential
Dotted line : $|\nabla V|$
Dashed line : $|\nabla^2 V|$

Figure 7a : ^{16}O
Figure 7b : ^{40}Ca.

FIGURE 7a)

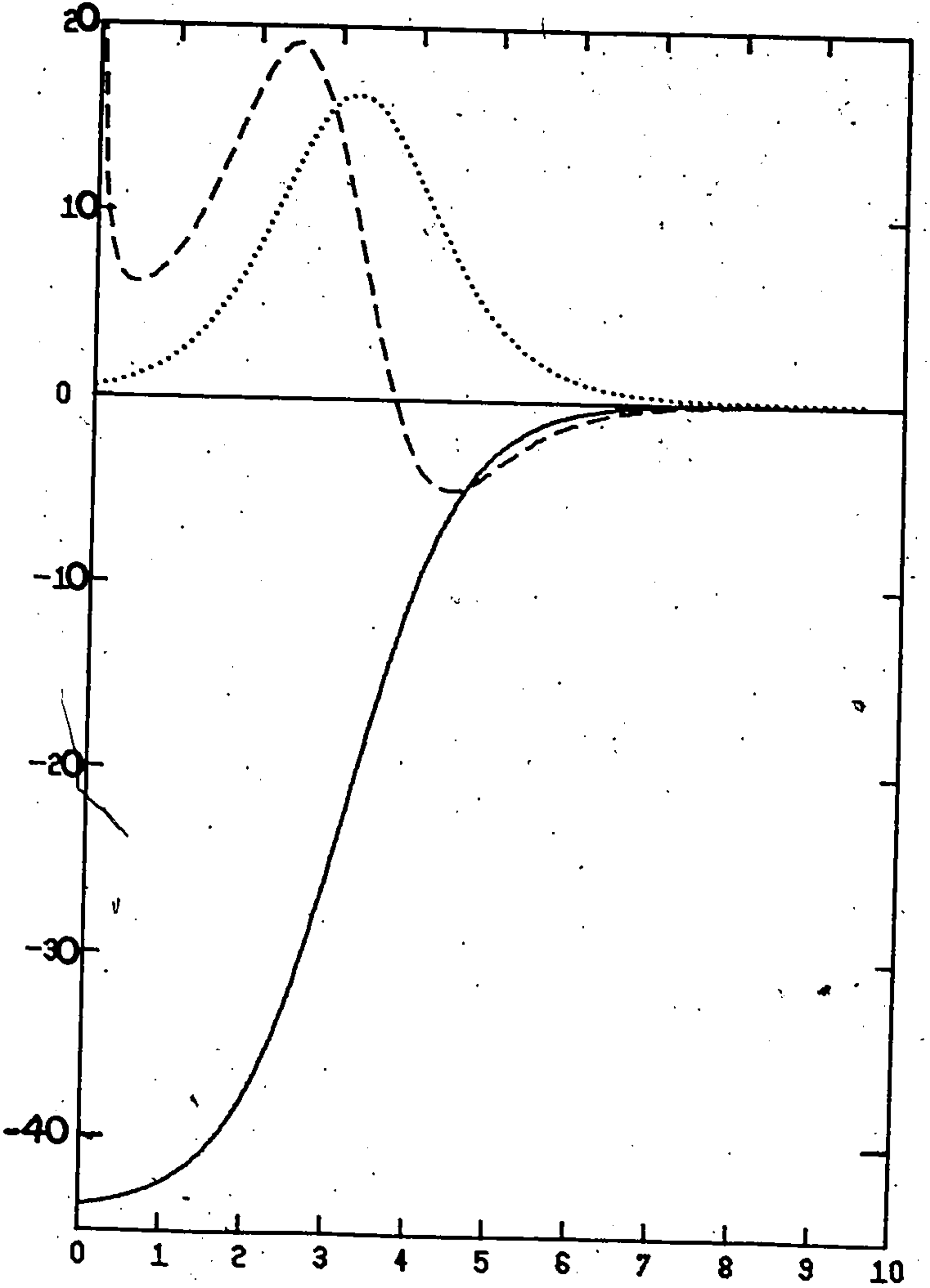
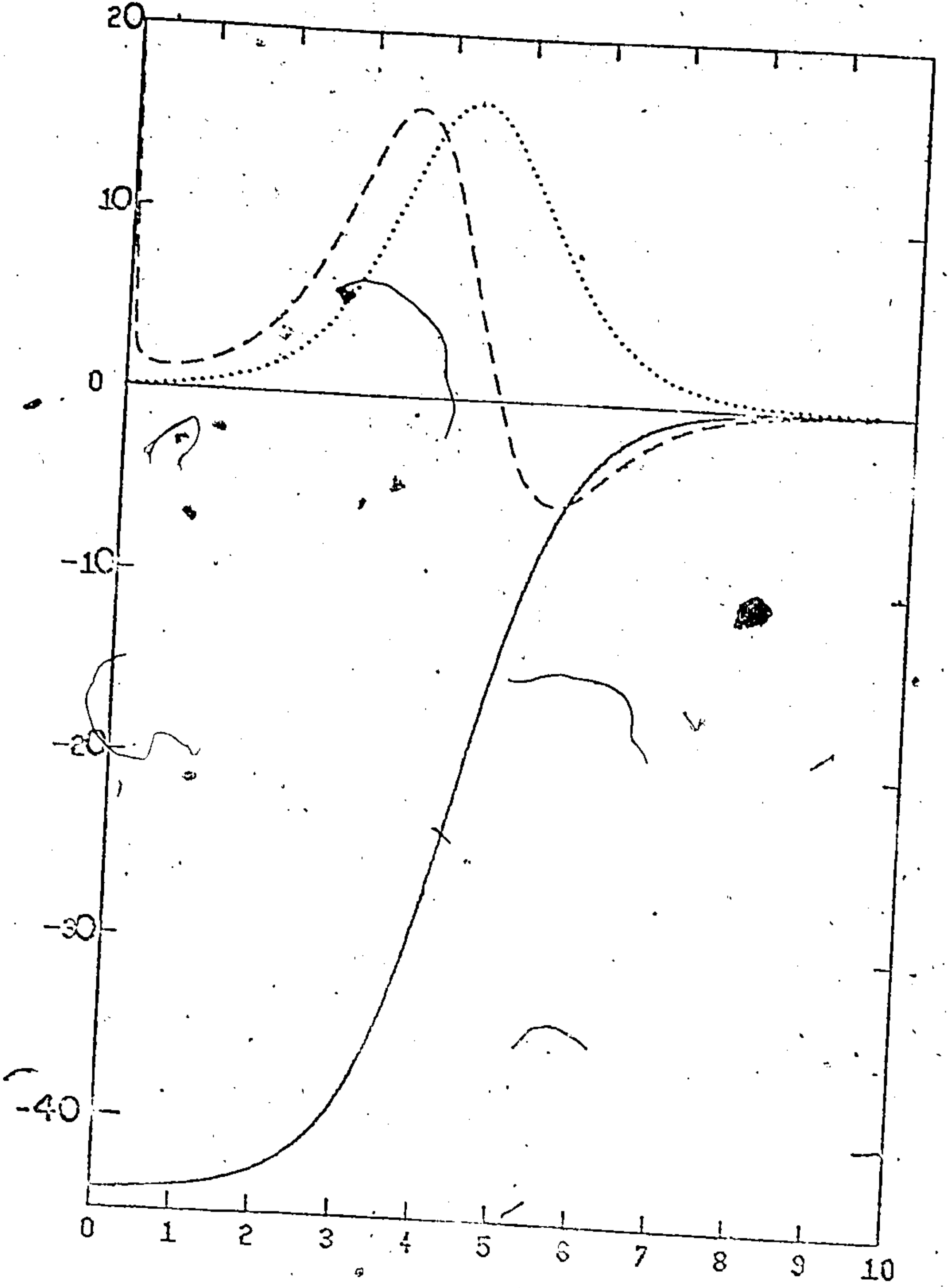


FIGURE 7 b)



Laplace invert to the Fermi energy (see chapter 1). Therefore we do not expect the approximation to give good results for excited states. It was found that the HOA did not reproduce $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}$ very well for spherically symmetric excited states, even in a harmonic oscillator potential.

iii) Discussion and Conclusion

We have shown that as a Taylor series expansion up to fourth order in $\underset{\sim}{S}$, the HOA is more accurate in the interior of the nucleus considered in a Woods Saxon potential than either the CBA or the NVA in 3 dimensions. In one dimension it was also reasonably accurate with the Eckart potential. As it is also exact for the harmonic oscillator potential, one might hope that this approximation would be very good for nuclear calculations. This is particularly hopeful in view of the fact that neither the Eckart potential nor the Woods Saxon potential have small high derivatives in the region over which the HOA is good. However, in its present form it is not a useful calculational tool.

Although the Taylor series gives the small S behaviour very well, the density matrix blows up very rapidly when S is greater than 2 fm (see figures 3) and 5)). Thus, even for a short range force such as a Yukawa with a range of 0.7 fm (for 2 pion exchange), the exchange integral will be very inaccurate if the calculation is done using a Taylor series expansion. This is basically because the process of interchanging summing of the series and integration is not legitimate over an infinite interval, since we don't have uniform convergence of the series on this interval.

This shows the necessity of including the long range S behaviour of the density matrix. One may hope that it is possible to write down a form for the density matrix whose Taylor series reproduces the HOA up to fourth order, and sums S up to infinite order, with higher than fourth order coefficients being undetermined. The simplest approach to this problem is to use the theory of Padé approximants (Baker, 1975) to estimate the long range behaviour of the density matrix.

Using a Taylor series expansion up to S^4, one can fix the asymptotic behaviour to be at most $\frac{1}{S^4}$. It was found that this did not produce enough damping to give an accurate result in the case of ^{4}He in a harmonic oscillator potential; for which $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}$ is known in closed form.

Some form must be proposed in which the long range behaviour in S is heavily damped so that reasonably accurate integrals may be calculated. In Negele-Vautherin's theory they expand in a plane wave basis and get Bessel functions for the form of the density matrix. It is the artificial damping introduced by the Bessel functions which allows the exchange integral to be calculated using their form. It may be possible to fix up the NVA to produce the HOA up to S^4 and still retain the Bessel function form for damping out the long range behaviour.

Another approach may be more successful than this. Since finite nuclei have wavefunctions which more closely resemble harmonic oscillator wavefunctions than plane waves, the harmonic oscillator basis may be a better basis for expansion of the density matrix. (1.48) sums up S to infinite order, but cannot be Laplace inverted analytically. If it could be approximated in a way which sums S up to infinite order, but may be Laplace inverted analytically we will have achieved this aim. Such a theory should probably reproduce the HOA up to a given order in S, with differing higher coefficients.

A second problem which hasn't been looked at in this thesis is the error introduced by assuming $\overline{\rho^2(\underset{\sim}{Q},\underset{\sim}{S})} = \overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}^2$ when calculating exchange integrals. It is really $\overline{\rho^2(\underset{\sim}{Q},\underset{\sim}{S})}$ which is needed in this calculation whereas the HOA approximates $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}$. It is easy to verify that beyond the S^2 term, all other coefficients differ. This difference has not been looked at numerically, so no quantitative results may be presented. However, if one looks at table II we can see that the S^4 coefficient of $\overline{\rho(\underset{\sim}{Q},\underset{\sim}{S})}$ is about 6% of the size of the S^2 coefficient. Thus, any difference in the S^4 coefficient of $\overline{\rho^2(\underset{\sim}{Q},\underset{\sim}{S})}$ due to the above not being equal must produce a small effect on the final result of an integral.

In conclusion, we have shown the HOA to be accurate in one and three dimensions, even for potentials not similar to the harmonic oscillator. Its accuracy, for a given potential, increases with particle number, and hence is appropriate for heavy nuclei. It will probably be the most accurate approximation for short range forces which die off before the 1/2 density radius, whereas the CBA is probably more accurate for intermediate and long range forces which extend beyond the 1/2 density radius. More work is needed to put the HOA in a form amenable to calculation.

APPENDIX A

THE DENSITY MATRIX FOR LINEAR AND QUADRATIC POTENTIALS

It is possible to show that the density matrix for the linear potential V = kx may also be written in the same form as (1.39). The wavefunctions for this potential are (Landau and Lifshitz, 1977):

$$\sqrt{\frac{k}{\pi}}\,\sigma \mathrm{Ai}(-\sigma(E-V(x))) = \sqrt{\frac{k}{\pi}}\,\frac{\sigma}{2\pi}\int_{-\infty}^{\infty} e^{i(t^3/3-\sigma(E-V(x))t)}dt \,. \qquad (1)$$

where Ai(x) is the Airy function and $\sigma = \left(\frac{2m}{\hbar^2 k^2}\right)^{1/3}$. Since the spectrum of the Hamiltonian is continuous, we must integrate the square of (1) to obtain the density.

$$\rho(q,s,\mu) = \frac{k}{\pi}\,\sigma^2 \int_0^{\mu} \mathrm{Ai}[-\sigma(E-kq-\frac{ks}{2})]\mathrm{Ai}[-\sigma(E-kq+\frac{ks}{2})]dE \,. \qquad (2)$$

We may rewrite (2) in a more convenient form by noting that (1) doesn't change under the transformation t → −t. Then we write:

$$\mathrm{Ai}[-\sigma(E-kq-\frac{ks}{2})]\mathrm{Ai}[-\sigma(E-kq+\frac{ks}{2})]$$

$$= \frac{1}{4\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i(\frac{1}{3}(t^3-t'^3)-\sigma(E-kq)(t-t')+\sigma\frac{ks}{2}(t+t'))}dtdt'. \qquad (3)$$

which becomes:

$$\frac{1}{4\pi^2}\int_{-\infty}^{\infty} e^{i\left(\frac{v^3}{12} - \sigma(E-kq)v\right)} \int_{-\infty}^{\infty} e^{-iv\frac{u^2}{4}} e^{-i\sigma\frac{ks}{2}u}\, du\, dv \qquad (4)$$

where $v = t-t'$, $u = t+t'$. A second change of variables, $v \rightarrow iv'$ produces

$$\frac{1}{2\pi^2 i}\int_{-i\infty}^{i\infty} e^{\frac{v'^3}{12} + \sigma(E-kq)v'} \int_{0}^{\infty} e^{-\frac{u^2 v}{4}} \cos\left(\frac{\sigma k s u}{2}\right) du\, dv\ . \qquad (5)$$

The u integral may be done analytically to yield:

$$\begin{aligned} &\mathrm{Ai}\left[-\sigma\left(E-kq-\frac{ks}{2}\right)\right]\mathrm{Ai}\left[-\sigma\left(E-kq+\frac{ks}{2}\right)\right] \\ &= \frac{1}{2\sqrt{\pi}} \cdot \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} e^{v\sigma(E-kq)}\, \frac{e^{\frac{v^3}{12} - \frac{\sigma^2k^2s^2}{}}}{\sqrt{v}} \\ &= \frac{1}{2\sqrt{\pi}}\, L^{-1}\left[\frac{e^{\frac{v^3}{12} - \frac{\sigma^2k^2s^2}{4v}}}{\sqrt{v}},\ v \rightarrow \sigma[E-kq]\right] \end{aligned} \qquad (6)$$

This allows us to write the density matrix:

$$\rho(q,s,\mu) = \frac{k\sigma^2}{2\pi^{3/2}}\int_{0}^{\mu} \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} e^{\frac{v^3}{12} + \sigma(E-kq)v}\, \frac{e^{-\frac{\sigma^2k^2s^2}{4v}}}{\sqrt{v}}\, dv\, dE\ . \qquad (7)$$

Since the off-diagonal terms are independent of the diagonal terms the expansion in s is trivial.

$$\rho(q,s,\mu) = \frac{k\sigma^2}{2\pi^{3/2}} \int_0^{\mu} \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \frac{e^{\frac{v^3}{12} + \sigma(E-kq)v}}{\sqrt{v}} \left(1 - \frac{\sigma^2 k^2 s^2}{4v} + \frac{\sigma^4 k^4 s^4}{32v^2} + \right.$$

$$\left. + (-)^n \frac{\sigma^{2n} k^{2n} s^{2n}}{n!\,4^n v^n} + \cdots \right) dv dE \; . \tag{8}$$

We may easily write the diagonal term by setting s=0 in (7).

$$\rho(q,\mu) = \frac{k\sigma^2}{2\pi^{3/2}} \int_0^{\mu} \frac{1}{2\pi i} \int_{-i\infty}^{\infty} \frac{e^{\frac{v^3}{12} + \sigma(E-kq)v}}{\sqrt{v}} dv dE$$

$$= \frac{k\sigma^2}{\pi} \int_0^{\mu} Ai^2[-\sigma(E-kq)]dE \; . \tag{9}$$

From (9) we can see that powers of $v^{-(n + \frac{1}{2})}$ may be generated by integration with respect to q.

$$\frac{1}{2\sqrt{\pi}} \frac{1}{2\pi i} \frac{e^{\frac{v^3}{12} + v\sigma(E-kq)}}{v^{n + \frac{1}{2}}} dv$$

$$= \frac{1}{2\sqrt{\pi}} \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \sigma^n \int_q^{\infty} \cdots \int_{x_{n-1}}^{\infty} \frac{e^{\frac{v^3}{12} + v\sigma(E-kx_n)}}{v^{n + \frac{1}{2}}} \frac{dV}{dx_n} dx_n \cdots \frac{dV}{dx_1} dx_1 dv \tag{10}$$

where $\frac{dV}{dx_i} = k$.

Then we have for the s^{2n} coefficient:

$$(-)^n \frac{(\sigma^3k^2)^n}{4^n n!} \int_q^\infty \cdots \int_{x_{n-1}}^\infty \frac{k\sigma^2}{\pi} \int_0^\mu Ai^2[-\sigma(E-kx_n)]dE \frac{dV}{dx_n} dx_n \cdots \frac{dV}{dx_1} dx_1 \ . \quad (11)$$

We may then reduce this to the form of (1.39) if we can show that

$$\frac{1}{2} \int_q^\infty \rho(x) \frac{dV}{dx} dx = \tau(q) - \frac{1}{4} \frac{\hbar^2}{2m} \frac{d^2\rho}{dq^2} \ .$$

To do this we write the Block density matrix:

$$C(q,s,\beta) = \frac{k\sigma^2}{2\pi^{3/2}} \int_0^\infty Ai[-\sigma(E-kg-\frac{ks}{2})]Ai[-\sigma(E-kq+\frac{ks}{2})]e^{-\beta E}dE$$

$$= \frac{k\sigma^2}{2\pi^{3/2}} \frac{e^{\frac{\beta^3}{12\sigma^3}}}{\sqrt{\sigma\beta}} e^{-\beta kq} e^{-\frac{\sigma^3k^2}{4\beta} s^2} \quad (12)$$

where the last line follows from (6) if one notes that (12) is a Laplace transform.

$$\tau(q,\beta) = \frac{\hbar^2}{2m} (\frac{\beta^2k^2}{4} + \frac{\sigma^3k^2}{2\beta}) \quad C(q,\beta). \quad (13)$$

$$\frac{d^2C(q,\beta)}{dq^2} = \beta^2k^2C(q,\beta) \quad (14)$$

$$\tau(q,\beta) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2C(q,\beta)}{dq^2} = \frac{\hbar^2}{2m}\frac{\sigma^3k^2}{2\beta} C(q,\beta). = \frac{1}{2}\int_q^\infty C(x,\beta) \frac{dV}{dx} dx \ . \quad (15)$$

We may note that $\sigma^3k^2 = (\frac{2m}{\hbar^2})$ and that (15) is linear in the transformed quantities to write (11) as:

$$(-)^n \frac{2(\frac{2m}{\hbar^2})^n}{4^n n!} \int_q^\infty \cdots \int_{x_{n-2}}^\infty (\tau(x_{n-1}) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2\rho}{dx_{n-1}^2}) \frac{dV}{dx_{n-1}} dx_{n-1} \cdots \frac{dV}{dx_1} dx_1 \quad (16)$$

and hence we write (2) as:

$$\rho(q,s,\mu) = \rho(q,\mu) - \frac{1}{2}\left(\frac{2m}{\hbar^2}\right)\left(\tau(q) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2\rho(q)}{dq^2}\right)s^2$$

$$+ \frac{1}{16}\left(\frac{2m}{\hbar^2}\right)^2 \int_q^\infty \left(\tau(x_1) - \frac{1}{4}\frac{d^2\rho(x_1)}{dx_1^{\,2}}\right)\frac{dV}{dx_1}\,dx_1\, s^4 + \cdots$$

$$+ (-)^n \frac{2\left(\frac{2m}{\hbar^2}\right)^n}{4^n n!} \int_q^\infty \cdots \int_{x_{n-2}}^\infty \left(\tau(x_{n-1}) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2\rho(x_{n-1})}{dx_{n-1}^2}\right)\frac{dV}{dx_{n-1}}\,dx_{n-1}\cdots\frac{dV}{dx_1}\,dx_1\, s^{2n}$$

$$+ \cdots . \qquad (17)$$

which is identical in form to (1.39).

It is also easy to show that the quadratic potential

$$V(x) = a + bx + cx^2$$

has the same form for its density matrix. The eigenfunctions are:

$$\psi_n(x) = \frac{\alpha}{\sqrt{2^n n!}\,(\pi)^{1/4}} H_n\left[\alpha\left(x + \frac{b}{2c}\right)\right] e^{-\frac{1}{2}\alpha^2\left(x + \frac{b}{2c}\right)^2} \qquad (19)$$

corresponding to the eigenvalue:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) + a - \frac{b^2}{4c} \qquad (20)$$

where we have written

$$\omega = \sqrt{\frac{2}{m}\, c} \quad , \qquad \alpha = \sqrt{\frac{m\omega}{\hbar}} = (\frac{2m}{\hbar^2}\, c)^{1/4} .$$

Then it is easy to write the Block Density matrix:

$$C^{\text{quad.}}(x,x',\beta) = e^{-\beta(a-\frac{b^2}{4c})} \frac{\alpha}{\sqrt{2\pi \sinh(\beta\hbar\omega)}} \exp(-\frac{\alpha^2}{2}\, \{(x^2+x'^2) + $$

$$+ \frac{b}{c}\,(x+x') + 2\frac{b^2}{4c^2})\coth(\beta\hbar\omega) - 2(xx' + \frac{b}{2c}(x+x') + \frac{b^2}{4c^2})\operatorname{csch}(\beta\hbar\omega)\}) . \tag{21}$$

and in q and s space we have:

$$C^{\text{quad.}}(q,s,\beta) = e^{-\beta(a-\frac{b^2}{4c})} \frac{\alpha}{\sqrt{2\pi \sinh(\beta\hbar\omega)}} \exp[-\alpha^2(q+\frac{b}{2c})^2 \tanh(\frac{\beta\hbar\omega}{2})]$$

$$\cdot \exp[-\alpha^2\, \frac{s^2}{4} \coth(\frac{\beta\hbar\omega}{2})] . \tag{22}$$

We now show that a relationship similar to (35) holds for (22). Note that $\frac{dV}{dx} = b + cx$. If we write $x' = x + \frac{b}{c}$, then we can integrate (22) in the following form:

$$\frac{1}{c}\, \frac{\alpha e^{-\beta(a-\frac{b^2}{4c})}}{\sqrt{2\pi \sinh(\beta\hbar\omega)}} \int_{q+\frac{b}{c}}^{\infty} \exp(-\alpha^2(x'-\frac{b}{2c})^2 \tanh(\frac{\beta\hbar\omega}{2})\, 2cx'dx'$$

$$= \frac{2m}{h^2}\, \frac{1}{2\alpha^2} \coth(\beta\hbar\omega)\, \frac{\alpha e^{-\beta(a-\frac{b^2}{4c})}}{\sqrt{2\pi \sinh(\beta\hbar\omega)}} \exp(-\alpha^2(q+\frac{b}{2c})^2 \tanh(\frac{\beta\hbar\omega}{2})) \tag{23}$$

where $2cx' = \frac{dV}{dx}$.

Again we can show a repeated integration gives higher powers of $\coth(\beta\hbar\omega)\ C^{\text{quad}}(q,\beta)$ similar to (1.37).

We can also write the transformed kinetic energy density:

$$\tau^{\text{quad}}(q,\beta) = \alpha^4 \left(q + \frac{b}{2c}\right)^2 C^{\text{quad}}(q,\beta) \tag{24}$$

and

$$\tau^{\text{quad}}(q,\beta) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2 C^{\text{quad}}(q,\beta)}{dq^2} = \frac{1}{2}\alpha^2 C^{\text{quad}}(q,\beta)$$

$$= \frac{1}{2}\int_q^\infty C^{\text{quad}}(x,\beta)\,\frac{dV}{dx}\,dx. \tag{25}$$

Hence, in analogy with (1.39) we write:

$$\rho^{\text{quad}}(q,s) = \rho^{\text{quad}}(q) - \frac{1}{2}\frac{2m}{\hbar^2}\left(\tau^{\text{quad}}(q) - \frac{1}{4}\frac{\hbar^2}{2m}\frac{d^2\rho^{\text{quad}}(q)}{dq^2}\right)s^2$$

$$+ \frac{1}{16}\left(\frac{2m}{\hbar^2}\right)^2 \int^\infty \left(\tau^{\text{quad}}(q)\,\frac{1}{4}\frac{h^2}{2m}\frac{d^2\rho^{\text{quad}}(q)}{dx}\right)\frac{dV}{dx}\,dx\cdot s^4 + \cdots \,. \tag{26}$$

APPENDIX B

ANGLE AVERAGING

In the independent particle approximation the density matrix is a sum over occupied states.

$$\rho(\underset{\sim}{Q},\underset{\sim}{S}) = \sum_{i=0}^{N} g_i \psi_i(\underset{\sim}{Q} + \frac{\underset{\sim}{S}}{2}) \psi_i^*(\underset{\sim}{Q} - \frac{\underset{\sim}{S}}{2}) \quad . \tag{1}$$

(see equation (1.1)).

The wavefunctions may be expanded in a Taylor series in the relative coordinate $\underset{\sim}{S}$.

$$\psi(\underset{\sim}{Q} + \frac{\underset{\sim}{S}}{2}) = \sum_{n=0}^{\infty} \frac{1}{2^n n!} (\underset{\sim}{S}\cdot\nabla)^n \psi(\underset{\sim}{Q}) \tag{2a}$$

$$\psi^*(\underset{\sim}{Q} - \frac{\underset{\sim}{S}}{2}) = \sum_{n=0}^{\infty} \frac{1}{2^n n!} (-)^n (\underset{\sim}{S}\cdot\nabla)^n \psi^*(\underset{\sim}{Q}) \quad . \tag{2b}$$

where the gradient acts only on the centre of mass coordinate.

Using (2), we may rewrite (1) in an expansion in powers of $\underset{\sim}{S}$ to obtain:

$$\begin{aligned} \rho(\underset{\sim}{Q},\underset{\sim}{S}) = \sum_{i=1}^{N} g_i \{ & \psi_i^*(\underset{\sim}{Q})\psi_i(\underset{\sim}{Q}) + \frac{1}{4}(\psi_i^*(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\nabla)^2\psi_i(\underset{\sim}{Q}) \\ & - \underset{\sim}{S}\cdot\underset{\sim}{\nabla}\psi_i^*(\underset{\sim}{Q})\underset{\sim}{S}\cdot\nabla\psi_i(\underset{\sim}{Q})) + \frac{1}{192}(\psi_i^*(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\nabla)^4\psi_i(\underset{\sim}{Q}) - \\ & - 4(\underset{\sim}{S}\cdot\nabla)\psi_i^*(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\nabla)^3\psi_i(\underset{\sim}{Q}) + 3(\underset{\sim}{S}\cdot\nabla)^2\psi_i^*(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\nabla)^2\psi_i(\underset{\sim}{Q})) + \cdots \} \quad . \end{aligned} \tag{3}$$

Since we are interested in cases where only the magnitude of $\underset{\sim}{S}$ is important, (3) must be angle-averaged over the direction of $\underset{\sim}{S}$. We denote the angle average of the quantity A by $\bar{A}$. Then we angle average using the following prescription:

$$\bar{A} = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} A(\theta,\phi)\sin\theta\, d\theta\, d\phi \ . \qquad (4)$$

In angle averaging (3), it is convenient to use momentum space wavefunctions (Flugge, 1974):

$$\psi(\underset{\sim}{Q}) = \frac{1}{(2\pi)^{3/2}}\int e^{i\underset{\sim}{k}\cdot\underset{\sim}{Q}} f(\underset{\sim}{k})\, d^3k \ . \qquad (5)$$

Then gradients become the vector $\underset{\sim}{k}$, and the procedure for angle averaging then becomes more clear.

We first set up a coordinate system:

i) $\underset{\sim}{k} = (k, \frac{\pi}{2}, 0)$

ii) $\underset{\sim}{k}' = (k', \frac{\pi}{2}, \gamma)$

iii) $\underset{\sim}{S} = (S, \theta, \phi)$ (6)

The following relation is useful in evaluating scalar products (Arfken, 1970).

$$\cos\beta = \cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\phi_1-\phi_2) \qquad (7)$$

where β is the included angle between two vectors of angular coordinates (θ_1,ϕ_1) and (θ_2,ϕ_2).

The scalar products in (3) are then easy to evaluate. To angle average the first term is trivial since there is no $\underset{\sim}{S}$ dependence.

$$\sum_{i=1}^{N} g_i \, \overline{\psi_i^*(\underset{\sim}{Q})\psi_i(\underset{\sim}{Q})} = \rho(\underset{\sim}{Q}) \ . \tag{8}$$

The next term contains two terms which need to be angle averaged:

$$\psi^*(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\nabla)^2\psi(\underset{\sim}{Q}) - \underset{\sim}{S}\cdot\nabla\psi^*(\underset{\sim}{Q})\underset{\sim}{S}\cdot\nabla\psi(\underset{\sim}{Q}) =$$

$$= \frac{1}{(2\pi)^3}\iint e^{i\underset{\sim}{Q}\cdot(\underset{\sim}{k}-\underset{\sim}{k}')} f(\underset{\sim}{k})f^*(\underset{\sim}{k}')((\underset{\sim}{S}\cdot\underset{\sim}{k})^2 - \underset{\sim}{S}\cdot\underset{\sim}{k}\underset{\sim}{S}\cdot\underset{\sim}{k}')d^3k\,d^3k' \ . \tag{9}$$

$$\overline{(\underset{\sim}{S}\cdot\underset{\sim}{k})^2} = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} \sin^3\theta d\theta \cos^2\phi d\phi S^2k^2 = \frac{1}{3}S^2k^2 \tag{10}$$

$$\overline{(\underset{\sim}{S}\cdot\underset{\sim}{k})(\underset{\sim}{S}\cdot\underset{\sim}{k}')} = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} \sin^3\theta d\theta\cos\phi(\cos\phi\cos\gamma+\sin\phi\sin\gamma)d\phi S^2kk'$$

$$= \frac{1}{3}\underset{\sim}{k}\cdot\underset{\sim}{k}'S^2 \ . \tag{11}$$

Hence in coordinate space we have:

$$\frac{1}{4}\sum_{i=1}^{N} g_i\overline{\{\psi_i^*(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\nabla)^2\psi_i(\underset{\sim}{Q})-\underset{\sim}{S}\cdot\nabla\psi_i^*(\underset{\sim}{Q})S\cdot\nabla\psi_i(\underset{\sim}{Q})\}}$$

$$=\frac{1}{12}S^2\sum_{i=1}^{N} g_i\{\psi_i^*(\underset{\sim}{Q})\nabla^2\psi_i(\underset{\sim}{Q})-\nabla\psi_i^*(Q)\cdot\nabla\psi_i(\underset{\sim}{Q})\}$$

$$=-\frac{1}{6}\frac{2m}{\hbar^2}\left(\tau(\underset{\sim}{Q})-\frac{1}{4}\frac{\hbar^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right)S^2. \qquad (12)$$

In the fourth order term we need to angle average:

$$\psi^*(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\underset{\sim}{\nabla})^4\psi(\underset{\sim}{Q})-4(\underset{\sim}{S}\cdot\underset{\sim}{\nabla})\psi^*(\underset{\sim}{Q})(\underset{\sim}{S}\cdot\underset{\sim}{\nabla})^3\psi(Q)+3(\underset{\sim}{S}\cdot\underset{\sim}{\nabla})^2\psi^*(Q)(\underset{\sim}{S}\cdot\underset{\sim}{\nabla})^2\psi(Q)$$

$$=\frac{1}{(2\pi)^3}\iint e^{i\underset{\sim}{Q}\cdot(\underset{\sim}{k}-\underset{\sim}{k}')}f(k)f^*(k')\{(\underset{\sim}{S}\cdot\underset{\sim}{k})^4-4(\underset{\sim}{S}\cdot\underset{\sim}{k}')(\underset{\sim}{S}\cdot\underset{\sim}{k})^3$$

$$+3(\underset{\sim}{S}\cdot\underset{\sim}{k})^2(\underset{\sim}{S}\cdot\underset{\sim}{k}')^2\}d^3k\,d^3k' \qquad (13)$$

$$\overline{(\underset{\sim}{S}\cdot\underset{\sim}{k})^4}=\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}\sin^5\theta d\theta\cos^4\phi d\phi S^4k^4=\frac{1}{5}S^4k^4 \qquad (14)$$

$$\overline{\underset{\sim}{S}\cdot\underset{\sim}{k}'(\underset{\sim}{S}\cdot\underset{\sim}{k})^3}=\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}\sin^5\theta d\theta\cos^3\phi(\cos\phi\cos\gamma+\sin\phi\sin\gamma)d\phi k'k^3S^4$$

$$=\frac{1}{5}\underset{\sim}{k}\cdot\underset{\sim}{k}'k^2S^4 \qquad (15)$$

$$\overline{(\underset{\sim}{S}\cdot\underset{\sim}{k})^2(\underset{\sim}{S}\cdot\underset{\sim}{k}')^2}=\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}\sin^5\theta d\theta\cos^2\phi\cos^2(\phi-\gamma)d\phi k'^2k^2S^4$$

$$=\frac{1}{5}\left(\frac{1}{3}k^2k'^2+\frac{2}{3}\underset{\sim}{k}\cdot\underset{\sim}{k}'\underset{\sim}{k}\cdot\underset{\sim}{k}'\right)S^4. \qquad (16)$$

Hence in coordinate space we have:

$$\frac{1}{960}\, s^4 \sum_{i=1}^{N} g_i \{ \psi_i(\underset{\sim}{Q}) \nabla^4 \psi_i(\underset{\sim}{Q}) - 4\nabla\psi_i^*(\underset{\sim}{Q}) \cdot \nabla\nabla^2 \psi_i(\underset{\sim}{Q})$$

$$+ \nabla^2\psi_i^*(\underset{\sim}{Q}) \nabla^2\psi_i(\underset{\sim}{Q}) + 2\nabla\nabla\psi_i^*(\underset{\sim}{Q}) : \nabla\nabla\psi_i(\underset{\sim}{Q}) \} \qquad (17)$$

where $\nabla\nabla$ is a rank 2 tensor operator and : indicates contraction across both indices.

In cartesian coordinates the tensor $\nabla\nabla$ is easy to write down; it has components $\frac{\partial^2}{\partial x_i \partial x_j}$. The contraction above is also easy

$$\nabla\nabla\psi^* : \nabla\nabla\psi = \sum_{i,j=1}^{3} \frac{\partial^2 \psi^*}{\partial x_i \partial x_j} \frac{\partial^2 \psi}{\partial x_i \partial x_j} . \qquad (18)$$

Upon performing the scalar products in (16) it is clear that (18) corresponds to the term $\underset{\sim}{k} \cdot \underset{\sim}{k}' \underset{\sim}{k} \cdot \underset{\sim}{k}'$ in momentum space. Since we are working with spherically symmetric systems, it would be convenient to obtain the tensor in a spherical basis. Since it is a symmetric tensor we reproduce the upper half only.

$$\nabla\nabla = \begin{bmatrix} \frac{\partial^2}{\partial r^2} & \frac{1}{r}\frac{\partial^2}{\partial\theta\partial r} - \frac{1}{r^2}\cdot\frac{\partial}{\partial\theta} & \frac{1}{r\sin\theta}\frac{2}{\partial r\partial\phi} - \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\phi} \\ & \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} & \frac{1}{r^2\sin\theta}\frac{\partial^2}{\partial\theta\partial\phi} - \frac{\cot\theta}{r^2\sin\theta}\frac{\partial}{\partial\phi} \\ & & \frac{1}{r}\frac{\partial}{\partial r} + \frac{\cot\theta}{r^2}\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin\theta}\frac{\partial^2}{\partial\phi^2} \end{bmatrix} \qquad (19)$$

In a system where the wavefunction is separable in a spherical coordinate system we write:

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_\ell^m(\theta,\phi) \tag{20}$$

where $R_{n\ell}(r)$ is the radial wavefunction, and $Y_\ell^m(\theta,\phi)$ is a spherical harmonic. Then we may use (19) and (20) to evaluate the term:

$$T4 = \nabla\nabla\psi^*(Q):\nabla\nabla\psi(Q) \tag{21}$$

in a spherical basis. We denote $\frac{d^2R_{n\ell}}{dr^2}$ by $R''_{n\ell}$, $\frac{dR_{n\ell}}{dr}$ as $R'_{n\ell}$.

$$\begin{aligned} T4 = {} & (R''^2_\ell + \frac{2}{r^2} R'^2_{n\ell})Y_\ell^m Y_\ell^{m*} + (2R'^2_{n\ell} + \frac{2}{r^2}\csc^2\theta R^2_{n\ell} - \frac{6}{r} R_{n\ell}R'_{n\ell}) \\ & \frac{m^2}{r^2\sin^2\theta} Y_\ell^m Y_\ell^{m*} + \frac{R^2_{n\ell}}{r^4\sin^4\theta} m^4 Y_\ell^m Y_\ell^{m*} + (\frac{2}{r^2} R'^2_{n\ell} - \frac{4}{r^3} R_{n\ell}R'_{n\ell} + \frac{1}{r^4} R^2_{n\ell} \\ & + \frac{\csc^2\theta}{r^4} R^2_{n\ell}) \frac{\partial Y_\ell^m}{\partial\theta} \frac{\partial Y_\ell^{m*}}{\partial\theta} + \frac{2R^2_{n\ell}}{r^4\sin^2\theta} m^2 \frac{\partial Y_\ell^m}{\partial\theta} \frac{\partial Y{m_\ell}^*}{\partial\theta} + \frac{4\cot\theta}{r^3} R_{n\ell}R'_n Y_\ell^{m*} \frac{\partial Y_\ell^m}{\partial\theta} \\ & - \frac{6\cot\theta R^2_{n\ell}}{r^4\sin^2\theta} m^2 Y_\ell^{m*} \frac{\partial Y_\ell^m}{\partial\theta} + \frac{2}{r^3} R_{n\ell}R'_{n\ell}Y_\ell^{m*} \frac{\partial^2 Y_\ell^m}{\partial\theta^2} + \frac{R^2_{n\ell}}{r^4} \frac{\partial^2 Y_\ell^{m*}}{\partial\theta^2} \frac{\partial^2 Y_\ell^m}{\partial\theta^2} . \end{aligned} \tag{22}$$

It would be most convenient to evaluate T4 if there were no angular dependence in it. Since we are mainly interested in working with filled shells, we find that summing over m for a fixed ℓ achieves this aim. Below we reproduce: $\sum_{m=-\ell}^{\ell}$ T4 for $\ell = 0$, $\ell = 1$, $\ell = 2$.

$$T4_0 = \frac{1}{4\pi} (R''^2_{n0} + \frac{2}{r^2} R'^2_{n0}) \tag{23}$$

$$T4_1 = \frac{3}{4\pi}\left(R''^2_{n1} + \frac{6}{r^2} R'^2_{n1} - \frac{12}{r^3} R_{n1}R'_{n1} + \frac{6}{r^4} R^2_{n1}\right) \qquad (24)$$

$$T4_2 = \frac{5}{4\pi}\left(R''^2_{n2} + \frac{14}{r^2} R'^2_{n2} - \frac{36}{r^3} R_{n2}R'_{n2} + \frac{42}{r^4} R^2_{n2}\right) . \qquad (25)$$

(23), (24) and (25) are valid for 1 particle per level. For the case in which they are g particles per level, we multiply T4 by g.

It is also possible to obtain the other terms in (17) without any angular dependence. To do this one notes that:

$$\sum_{m=-\ell}^{\ell} \nabla\psi^*_{n\ell m}\cdot\nabla\psi_{n\ell m} = \frac{2m}{\hbar^2}\tau_{n,\ell} \qquad (26)$$

and also makes use of Schrödinger's equation to obtain:

$$\frac{S^4}{960}\Big\{\frac{2m}{\hbar^2}(\rho\nabla^2 V + \nabla\rho\cdot\nabla V) + \left(\frac{2m}{\hbar^2}\right)^2 \sum_{n,\ell} (V-\varepsilon_{n,\ell})^2 R^2_{n\ell}\,\frac{2\ell+1}{\pi}$$

$$- 4\left(\frac{1}{2}\,\frac{2m}{\hbar^2}\nabla\rho\cdot\nabla V + \left(\frac{2m}{\hbar^2}\right)^2 \sum_{n,\ell} (V-\varepsilon_{n,\ell})\tau_{n,\ell}\right)$$

$$+ \left(\frac{2m}{\hbar^2}\right)^2 \sum_{n,\ell} (V-\varepsilon_{n\ell})^2 R^2_{n\ell}\,\frac{2\ell+1}{\pi} + 2\sum_{n,\ell,m} T4\Big\} \qquad (27)$$

where V is a spherically symmetric potential.

Then to fourth order in S we can write the angle average of (3) as:

$$\rho(\underset{\sim}{Q},\underset{\sim}{s}) = \rho(\underset{\sim}{Q}) - \frac{1}{6}\frac{2m}{\hbar^2}\left(\tau(\underset{\sim}{Q}) - \frac{1}{4}\frac{h^2}{2m}\nabla^2\rho(\underset{\sim}{Q})\right)s^2$$

$$+ \frac{1}{960}\left\{\frac{2m}{\hbar^2}\left(\rho(\underset{\sim}{Q})\nabla^2 V(\underset{\sim}{Q}) - \nabla\rho(\underset{\sim}{Q})\cdot\nabla V(\underset{\sim}{Q})\right) + \left(\frac{2m}{h^2}\right)^2 \sum_{n,\ell}\left(2(V(\underset{\sim}{Q})-\varepsilon_{n,\ell})^2\right.\right.$$

$$\left.\left. R_{n\ell}^2(\underset{\sim}{Q})\,\frac{2\ell+1}{\pi} - 4(V(\underset{\sim}{Q})-\varepsilon_{n,\ell})\tau_{n,\ell}(\underset{\sim}{Q})\right) + 2\sum_{n,\ell,m}\nabla\nabla\psi^*_{n\ell m}(\underset{\sim}{Q}):\nabla\nabla\psi_{n\ell m}(\underset{\sim}{Q})\right\}s^4$$

$$+ \cdots . \qquad (27)$$

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