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Correlation Effects in Nuclear Densities*

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Corrections to nuclear densities arising from static short-range correlations are evaluated for the nuclei ^{16}O, ^{40}Ca, and ^{56}Ni. The corrections are calculated using Rayleigh-Schrödinger perturbation theory in a basis obtained using Hartree-Fock. All corrections which are second order in the interaction are treated. The effects of necessary truncations are studied and are shown to render the results uncertain by about 20%. The net change in the density is a radial function which is less than 6% of the Hartree-Fock density and which oscillates in such a way that its effect on the rms radius is negligible. It is pointed out that in Brueckner-Hartree-Fock calculations a certain lack of cancellation might result in an excessively large change in the density and radius.

[NUCLEAR STRUCTURE calculated ρ and rms radius. Hartree-Fock plus second-order corrections.]

1. INTRODUCTION

Because the nucleon-nucleon interaction is not entirely known theoretically, numerous potentials, which are to some degree consistent with scattering data, are presently employed in many-nucleon problems. Whether or not the particular potential chosen for a calculation has an infinitely repulsive core, it is apparent that the nucleus does exhibit short-range two-body correlations. In order to take these correlations into account, an extensive theory based on the Bethe-Goldstone equation has been developed.[1] While such a theory does renormalize the interaction so that correlation effects are included in the calculated energy, present calculations of the density are still carried out using a single determinant.[2]

Investigations of the corrections to such a first-order density calculation, such as those of Negele,[3] indicate that higher-order corrections, i.e., the contribution from higher-order diagrams, are small, at least for the rms radius. Therefore in determining the parameters of an effective interaction, meant to represent the renormalized two-body potential, the results of electron scattering experiments, for example, are compared with single-determinant results.

A rather different approach consists of choosing a representation of the scattering data which is sufficiently "soft" so that straightforward perturbation expansions will converge. Then, instead of using the Bethe-Goldstone theory, one may apply the usual Rayleigh-Schrödinger perturbation theory with the Hartree-Fock method providing a basis. Such calculations have been carried out for the binding energies of the light spherical nuclei.[4]

The motivation of the present work, in which correlation effects on quantities other than the binding energy are calculated, is twofold. First, it is of interest to ascertain whether simple Hartree-Fock with second-order perturbation corrections can describe other properties of the nucleus as well as it does the energy. In fact it is quite likely that the perturbation series for the density is actually more rapidly convergent than the energy. This is so because the density is only a one-body operator whereas the energy contains two-body operators. This does not contradict the usual statement that the energy converges better than the wave function itself since that contains the N-particle density matrix, which is much more complicated than the Hamiltonian. Secondly, by performing such calculations one may examine the validity of the single-determinant approximation within the general context.

In the following section the perturbation expan-

sion for the one-particle density will be studied. In Sec. 3 the effect of truncating the infinite sums will be considered and in Sec. 4 the numerical results will be presented.

2. EXPANSION OF THE ONE-PARTICLE DENSITY

Hartree-Fock calculations have been performed using the Tabakin[5] interaction in a large variational space, neglecting the Coulomb interaction.[6] Single-particle energies and wave functions are given by the solutions of the Hartree-Fock equation:

$$\langle i|t|j\rangle + \sum_m \langle im|v|jm\rangle = \delta_{ij}\epsilon_i , \tag{1}$$

where $\langle im|v|jm\rangle$ is an antisymmetrized matrix element of the potential, $\langle i|t|j\rangle$ denotes one-particle kinetic energy matrix elements, and basis states m, a, and i are, respectively, hole states, particle states, and either of the two. Corresponding to these states, which are linear combinations of harmonic-oscillator eigenfunctions, are creation and destruction operators $a_i^\dagger$, a_i. In the space defined by these operators, the one-particle density operator has the form

$$\rho = \sum_{ij}\langle i|\rho|j\rangle a_i^\dagger a_j \equiv \sum_{ij}\rho_{ij}a_i^\dagger a_j$$

or, introducing the normal product relative to the Hartree-Fock (HF) ground state,

$$\rho = \rho_0 + \sum_{ij}\rho_{ij}:a_i^\dagger a_j: . \tag{2}$$

Here ρ_0 is the density in the HF determinant.

It is rather straightforward to calculate the expectation value of ρ in the wave function consisting of the HF ground state, $|0\rangle$, plus the first- and second-order perturbation corrections, $|1\rangle$ and $|2\rangle$. Retaining only terms up to second order in the interaction one obtains

$$\rho = \rho_0 + \Delta\rho_{02} + \Delta\rho_{11} , \tag{3}$$

where

$$\rho_0 = \langle 0|\rho|0\rangle ,$$

$$\Delta\rho_{02} = \langle 0|\rho|2\rangle = \Delta\rho_a + \Delta\rho_b ,$$

and

$$\Delta\rho_{11} = \langle 1|\rho|1\rangle = \Delta\rho_c + \Delta\rho_d . \tag{4}$$

Here the only contributions come from two-particle two-hole states in $|1\rangle$ and from one-particle one-hole states in $|2\rangle$. The various corrections to the density can be written as

$$\Delta\rho_g(\vec{r}) = \sum_{ij} d_{ij}^{(g)}\rho_{ij}(\vec{r}) , \tag{5}$$

for g = a, b, c, and d, where

$$d_{ma'}^{(a)} = \sum_{a,b,n}\frac{\langle mn|v|ab\rangle\langle ab|v|a'n\rangle}{(\epsilon_m-\epsilon_a')(\epsilon_m+\epsilon_n-\epsilon_a-\epsilon_b)} ,$$

$$d_{am'}^{(b)} = \sum_{m,n,b}\frac{\langle ab|v|mn\rangle\langle mn|v|m'b\rangle}{(\epsilon_a-\epsilon_{m'})(\epsilon_m+\epsilon_n-\epsilon_a-\epsilon_b)} ,$$

$$d_{mm'}^{(c)} = -\frac{1}{2}\sum_{a,b,n}\frac{\langle mn|v|ab\rangle\langle ab|v|m'n\rangle}{(\epsilon_m+\epsilon_n-\epsilon_a-\epsilon_b)(\epsilon_m+\epsilon_n-\epsilon_a-\epsilon_b)} ,$$

$$d_{aa'}^{(d)} = \frac{1}{2}\sum_{m,n,b}\frac{\langle ab|v|mn\rangle\langle mn|v|a'b\rangle}{(\epsilon_m+\epsilon_n-\epsilon_a-\epsilon_b)(\epsilon_m+\epsilon_n-\epsilon_{a'}-\epsilon_b)} . \tag{6}$$

The HF contribution to the density can also be written in this form as

$$\rho_0 = \sum_{mm'} d_{mm'}^0\rho_{mm'} = \sum_m \rho_{mm} . \tag{7}$$

The HF term and the perturbation corrections are shown diagrammatically in Fig. 1.

The d coefficients thus defined are the components of the density matrix. From them one may immediately obtain the one-particle occupation probabilities P, including corrections to order v^2. Thus

$$P_m = 1 + d_{mm}^{(c)} ,$$

$$P_a = d_{aa}^{(d)} . \tag{8}$$

for the hole and particle states, respectively.

3. EFFECTS OF NUMERICAL TRUNCATION

Although there are alternative methods for evaluating $\Delta\rho_c$, $\Delta\rho_d$, and κ,[7] these as well as $\Delta\rho_a$ and

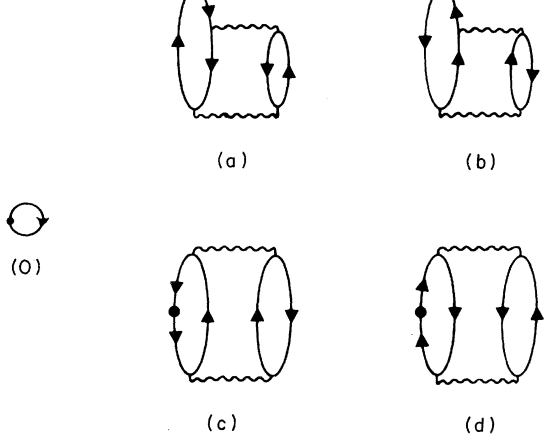

FIG. 1. Diagrammatic representation of the Hartree-Fock density and the second-order perturbation corrections to it. The letters (a)—(d) refer to the indices on the various $\Delta\rho$ terms in Eqs. (5) and (6).

$\Delta\rho_b$ may be explicitly and directly evaluated in the HF basis. The advantage to this method is that all terms and all parts of the interaction are treated uniformly rather than using different approximations appropriate for the central and tensor parts of the force or for the different geometries of the diagrams.

The difficulty with such a procedure arises from truncation. First of all, the single-particle orbitals are expanded in a large, but not of course infinite, basis and secondly, the total number of orbitals obtained by solving Eq. (6) must be truncated.

For the first point, the particle-state wave functions appear in two different ways: as matrix elements of the potential, which is short-range, and as representatives of the density operator, which, for light nuclei, have a range of interest of only a few fermis. Therefore, as with hole states, one needs to know these wave functions accurately over a relatively small distance. In this particular application the wave functions are described, with sufficient accuracy, up to at least 6 fm,[8] so that this truncation is of little consequence.

For the following it is of interest to consider the average change in the occupation probabilities, defined by

$$\kappa = \sum_m \frac{(1-P_m)}{A} = \sum_a \frac{P_a}{A}$$

$$= \frac{1}{2a} \sum_{mn} \sum_{ab} \left| \frac{\langle mn|v|ab\rangle}{\epsilon_m + \epsilon_n - \epsilon_a - \epsilon_b} \right|^2 . \tag{9}$$

This parameter is equivalent to the nuclear matter defect parameter which measures the strength of the short-range correlations. It is related to the magnitudes of the diagrams 1(c) and 1(d) through the equalities

$$\int d^3r \Delta\rho_c = \sum_{mm'} d^{(c)}_{mm'} \int d^3r \rho_{mm'} = -\kappa A$$

and

$$\int d^3r \Delta\rho_d = \sum_{aa'} d^{(d)}_{aa'} \int d^3r \rho_{aa'} = \kappa A \tag{10}$$

so that the fractional change in the density arising from each of these terms is of the order of κ. It may also be noted that diagrams (c) and (d) are each related to the square of the "defect function" and therefore arise from the same type of physical correlations which produce the g matrix.[9] Furthermore these diagrams approximately cancel each other in the calculation of the corrections to the rms radius in a finite nucleus.[7]

Although no analogous relationships exist for diagrams (a) and (b) it will be shown that a similar cancellation does occur. These diagrams prove to be of the same magnitude as (c) and (d), although the integrals of $\Delta\rho_a$ and $\Delta\rho_b$ are zero by virtue of the ρ indices being a particle and a hole.

In order to study the results of truncating the space it is convenient to introduce a parameter which will characterize the space. The use of $N\hbar\omega$ for such a purpose is inappropriate since it is the eigenvalues of the HF Hamiltonian, not the harmonic oscillator, one wishes to characterize. The parameter chosen is defined by

$$\xi = \frac{1}{M} \sum_{i=1}^{M} \epsilon_i , \tag{11}$$

where the set M is restricted to a single parity and to the highest HF state of a given set of quantum numbers, j and l. (Since only spherical nuclei are considered, only states with the same j and l are needed in the expansion of the HF states and there is complete degeneracy in j_z.) The set of states obtained by solving Eq. (1) in a space of N oscillator shells is called the model space which will henceforth be characterized by ξ.

The various quantities can now be considered to consist of two parts. For example, one may calculate a quantity $\kappa(\xi)$ with all sums limited to the model space,

$$\kappa(\xi) = \frac{1}{2A} \sum_{a,b \le \xi} \sum_{mn} \left| \frac{\langle mn|v|ab\rangle}{\epsilon_m + \epsilon_n - \epsilon_a - \epsilon_b} \right|^2 . \tag{12}$$

The remainder will be

$$\Delta\kappa(\xi) = \frac{1}{A} \sum_{\substack{a>\xi \\ b<\xi}} \sum_{mn} \left| \frac{\langle mn|v|ab\rangle}{\epsilon_m + \epsilon_n - \epsilon_a - \epsilon_b} \right|^2$$

$$+ \frac{1}{2A} \sum_{a,b>\xi} \sum_{mn} \left| \frac{\langle mn|v|ab\rangle}{\epsilon_m + \epsilon_n - \epsilon_a - \epsilon_b} \right|^2 . \tag{13}$$

Using a simple model one can estimate the remainder, $\Delta\kappa$, for a given model space computation. For large model spaces, in which particle states extend about 80 MeV into the continuum, the second term on the right-hand side of Eq. (13) is obviously small compared to the first and can be neglected. For the first term, following Kerman and Pal,[10] one makes the approximations:
(1) The particle states a, b are replaced by plane waves which are subsequently transformed to relative and center-of-mass momenta, $|ab\rangle = |\vec{K}\vec{k}\rangle$.
(2) The summation on a, b, is replaced by integrals over $\vec{K}$ and $\vec{k}$.
(3) The hole-state energies are replaced by an average value, $\epsilon_m + \epsilon_n \Rightarrow -2\Delta$.
(4) A multiplicative factor which roughly corrects for the phase space of the filled Fermi sea is in-

cluded

$$Q(K,k,k_f)=\begin{cases}0 & \text{if } k^2+\frac{1}{4}K^2<k_f{}^2,\\ 1 & \text{if } k-\frac{1}{2}K>k_f,\\ \dfrac{k^2+\frac{1}{4}K^2-k_f{}^2}{kK} & \text{otherwise.}\end{cases}$$

With these approximations Eq. (13) becomes

$$\Delta\kappa(\xi)=\frac{1}{A}\sum_{mn}\langle mn-nm|F|mn-nm\rangle, \tag{14}$$

where

$$F(\xi)=\int_{|k|>\sqrt{2}q} d^3Kd^3k\,\frac{v|\vec{K}\vec{k}\rangle Q(K,k,k_f)\langle\vec{K}\vec{k}|v}{[(\hbar^2/2m)(\frac{1}{2}k^2+\frac{1}{4}K^2)+2\Delta]^2} \tag{15}$$

and

$$q=\left(\frac{2m\xi}{\hbar^2}\right)^{1/2}.$$

For ^{16}O, in a model space given by $\xi=80$ MeV and choosing $\Delta=25$ MeV and $k_f=1.4$ fm^{-1}, the result is $\Delta\kappa(80)=0.017$ while $\kappa(80)=0.068$. It is therefore concluded that for this space, errors of approximately 20% are introduced by truncating the space, i.e., that $\kappa\simeq0.085$.

It should be noted that this value for κ is not so much smaller than that obtained from very much harder interactions.[11] This indicates that the contributions to κ come to a large extent from the lower energy region (below $\xi\simeq80$ MeV) even for those interactions.

To further examine this truncation effect one may fit the expression for $\kappa(\xi)$ in ^{16}O with the form

$$\kappa(\xi)=0.085-0.112\,e^{-0.026\Delta}\int_{t_0}^{\infty}dt\,\frac{e^{-t}}{t}, \tag{16}$$

where

$$t_0=7(\xi+3\Delta)/800. \tag{17}$$

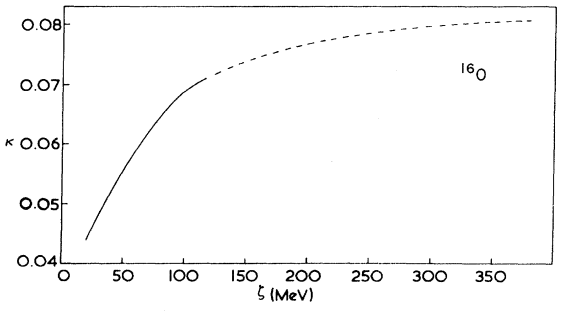

FIG. 2. Defect parameter κ in the ^{16}O as a function of the upper bound of the continuum. The solid curve represents explicit model space computations while the dashed curve is an extrapolation based on a simple Fermi-gas model.

The results are shown in Fig. 2. The solid line represents the results of a series of different model space calculations of $\kappa(\xi)$ for $\xi<80$ and the dashed curve the estimates obtained using Eq. (16). By construction the curves meet the 80 MeV. The fact that the curves continue smoothly through $\xi=80$ indicates methods are equally appropriate in the region of the intersection.

4. RESULTS: DENSITY AND rms RADIUS

Calculations of the corrections to the density were carried out for the nuclei ^{16}O, ^{40}Ca, and ^{56}Ni in a model space with $\xi=80$ MeV. The results are shown in Figs. 3–5. The solid curves, labeled a–d, represent the contributions of the four diagrams described in Sec. 2. The total second-order correction is also shown and labeled $\Delta\rho$. Since all of the corrections have a magnitude of the order of $\kappa\rho_0$, this quantity, $\pm\kappa\rho_0$, has been included in each figure. As the figures indicate, $\Delta\rho_a$ and $\Delta\rho_b$ are about as large as $\Delta\rho_c$ and $\Delta\rho_d$.

The main result of these calculations of the den-

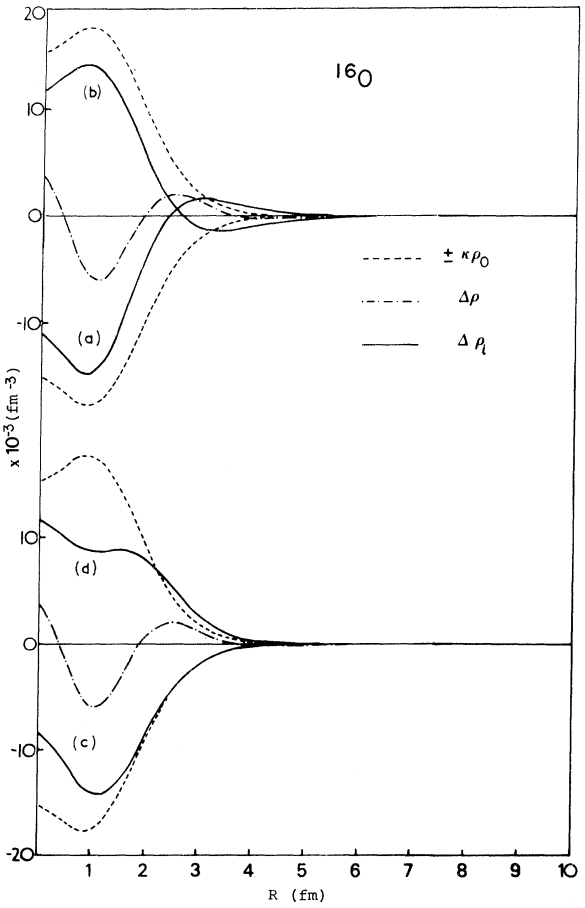

FIG. 3. Comparison of the terms $\Delta\rho_i$, $\pm\kappa\rho_0$, and $\Delta\rho$ in ^{16}O.

sity corrections is shown in Fig. 6. The three upper curves are the HF or single-determinant densities, ρ_0. The lower curves are the total second-order corrections, multiplied by 10 to show their structures. As is apparent from the figure, the total correction to the density is, at every point, smaller than 6%.

Having obtained the corrections to the density it is straightforward to calculate the change in rms radius a. Including second-order corrections the rms radius is given by

$$a = a_0\left(1 + \sum_i f_i\right), \tag{18}$$

where

$$a_0 = \left[\frac{1}{A}\int d^3r\, r^2 \rho_0(\vec{r})\right]^{1/2}, \tag{19}$$

and

$$f_i = \frac{1}{2a_0^2 A}\int d^3r\, r^2 \Delta\rho_i(\vec{r})\,. \tag{20}$$

TABLE I. Excitation parameter, rms radius, and fraction change in the rms radius.

	n	a_0	f_a	f_b	f_c	f_d	$\sum_i f_i$
^{16}O	0.068	2.38	0.031	−0.044	−0.035	0.044	−0.004
^{40}Ca	0.080	2.90	0.032	−0.034	−0.046	0.055	+0.007
^{56}Ni	0.081	2.98	0.022	−0.012	−0.032	0.040	+0.018

As is shown in the table the f_i's are not negligible and $a_0 f_i$ represents a correction to the rms radius of from 1 to 5% with varying signs. Because of this sign variation the net change in the radius is quite small, less than 1% in ^{16}O and ^{40}Ca and less than 2% in ^{56}Ni.

5. CONCLUSIONS

The second-order corrections to the density and rms radii of various nuclei have been calculated in a large model space. These corrections are in every case rather small indicating that single-determinant approximations are reasonable provided

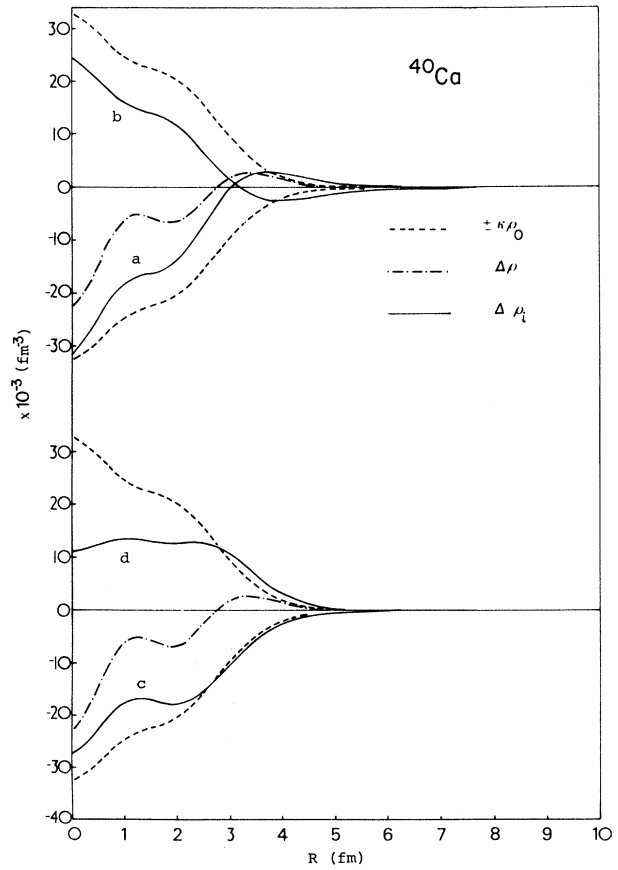

FIG. 4. Comparison of the terms $\Delta\rho_i$, $\pm\kappa\rho_0$, and $\Delta\rho$ in ^{40}Ca.

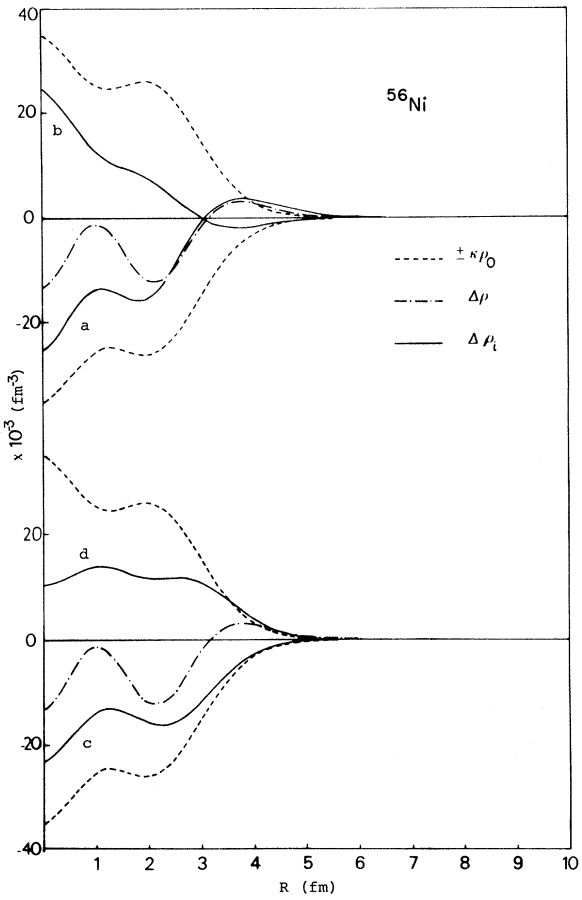

FIG. 5. Comparison of the terms $\Delta\rho_i k$, $\pm\kappa\rho_0$, and $\Delta\rho$ in ^{56}Ni.

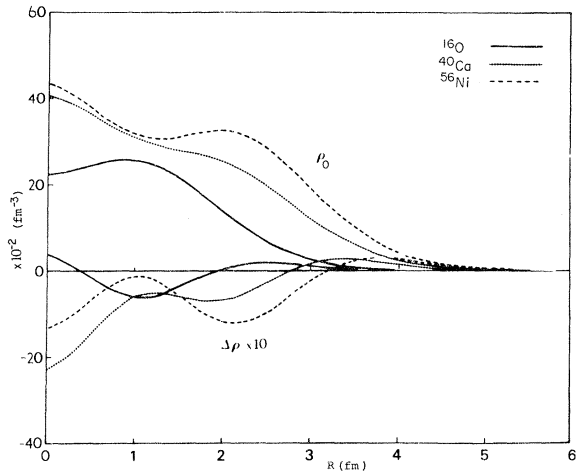

FIG. 6. Comparison of the density term ρ_0 and the correction term $\Delta\rho$.

all parts of the corrections are treated consistently.

The convergence of the calculation has been studied and, as is indicated by the calculation of κ, these results are uncertain by at most 20%. Since the size of the corrections does depend on a cancellation it is possible that this percent error will be multiplied in the final result. However, this will not change the conclusion that the second-order corrections are rather small. The quantity κ is sensitive to the details of the nucleon-nucleon interaction and it is known that "harder" potentials lead to larger values.

Independent of the particular interaction it appears that short-range correlations do not have a dramatic effect on the nuclear density. The corrections have the magnitude of $\kappa\rho_0$, with κ an average defect factor, and the different terms combine to have a small total value.

Finally, it is interesting to speculate on the outcome of similar computations using g matrices derived from strong potentials. In the calculations of Davies *et al.*[12] the average field is defined by solving the Brueckner-Hartree-Fock (BHF) equations. This gives single-particle and -hole wave functions quite similar to those resulting from HF calculations with the Tabakin interaction and they will be considered, in what follows, as identical. In the BHF theory the particle-hole potential is usually defined so that diagram 1(b) is exactly cancelled. Thus the terms contributing to the density, to this order, are 1(a) which is $-\kappa\rho_0$ and 1(c) and 1(d) which roughly cancel. In their calculations a κ of about $\frac{1}{6}$ would consequently decrease the central densities by about 15% and increase the radii by about 8%, if the diagram itself is not very small. In other calculations with nuclear matter g matrices, using the local density approximation, it is not clear that the diagram in Fig. 1(b) would be exactly cancelled so that no conclusion can be drawn. It would thus be of interest to have higher-order calculations of the density in the g-matrix framework.

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