Many-body perturbation calculation of spherical nuclei with a separable monopole interaction

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We present calculations of ground state properties of spherical, doubly closed-shell nuclei from ^{16}O to ^{208}Pb employing the techniques of many-body perturbation theory using a separable density-dependent monopole interaction. The model gives results in Hartree-Fock order that are of similar quality to other effective density-dependent interactions. In addition, second and third order perturbation corrections to the binding energy are calculated and are found to contribute small, but non-negligible corrections beyond the mean-field result. The perturbation series converges quickly, suggesting that this method may be used to calculate fully correlated wave functions with only second or third order perturbation theory. We discuss the quality of the results and suggest possible methods of improvement.

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I. INTRODUCTION

The central problem of nuclear structure theory is the solution of the many-body Schrödinger equation (MBSE). For Hamiltonians of interest in the nuclear case, an analytic solution is impossible and one is compelled to use some approximation, either in the numerical solution of the equation or the specification of the Hamiltonian, or both.

Approaching the problem with the aim of using as realistic a representation of the potential as possible usually means fitting a combination of a meson exchange and phenomenological interactions to low-energy nucleon-nucleon scattering data and properties of few-body systems. To get good agreement with experiment both two- and three-body forces seem to be necessary. Recent examples of such potentials include the Bonn [1], the Argonne two-body [2] with Urbana three-body [3], Nijmegen [4], and Moscow [5] potentials, the last of which also incorporates quark degrees of freedom. These forces share the property of having a hard repulsive core that is a natural consequence of meson exchange. It is this hard core that presents the difficulty in solving the MBSE. For instance, Hartree-Fock (HF) mean-field calculations with such interactions result in unbound nuclei. Treating corrections beyond the HF approximation order-by-order in perturbation theory is also unsuccessful since the interactions used are nonperturbative. One has to solve the full MBSE numerically in as exact a way as possible using techniques such as variational Monte Carlo [6], Green's function Monte Carlo (GFMC) [7], the coupled-cluster method [8,9], or the fermion hypernetted chain model [10]. Using effective interactions derived from realistic potentials, no-core shell-model calculations have been made in light nuclei [11], and heavier nuclei close to closed shells have been treated [12].

The computational difficulty of performing numerically exact solutions of the MBSE has limited the techniques to light nuclei, for instance $A=8$ results have been published recently using the Argonne $v18$ and Urbana IX potentials in the GFMC framework [13]. In this work, it is seen that although the lightest nuclei are reproduced very well, the quantitative comparison of theory to data gets worse as A increases. This may be due to the necessarily phenomenological nature of the three-body potential, a problem that may be overcome with refitting. On the other hand, it is not obvious that either higher-body forces will not prove necessary or that the concept of a bare interaction between nucleons is valid for small distances.

Attempts were made in the late 1960s primarily by Kerman and co-workers at MIT to parametrize the nucleon-nucleon interaction in such a way that it is weak in the sense of being perturbative, while still providing a good fit to scattering data. Such a weak interaction allows one to perform Hartree-Fock calculations to obtain a reasonable approximation to the full wave function and then to calculate corrections in perturbation theory. While this technique seems very attractive, the results obtained were only moderately successful at reproducing experimental data [14–18], a fact that was presumed to be due to inadequacies in the potentials used. The efficacy of developing a suitable interaction when similar, though more complicated techniques were available for realistic interactions has been questioned [19] and no better interaction was developed. Separable parametrizations, particularly the quadrupole-quadrupole force [20,21], have however retained currency as residual interactions [22]. Even when the potentials are too strong for regular perturbation theory, separable interactions requiring a solution of Brückner Hartree-Fock equations have proved fruitful [23] because of their simplicity.

On the other hand, interactions have been developed that are not intended for use in the full MBSE, but rather to give good results with a mean-field calculation alone. Good quantitative success came with the zero-range density-dependent force of Ehlers and Moszkowski [24] and Skyrme's interac-

tion [25], used in HF calculations by Vautherin and Brink [26] and subsequently by many others, and also Decharge and Gogny's finite-range interaction [27]. Skyrme's interaction has been particularly successful, in part due to its simple form, that of a delta function, which leads to easy calculation, even of the exchange part of the force. This computational simplicity has allowed extensive study of the properties of nuclei to be made with the Skyrme interaction across the entire range of nuclei in the periodic table [28–30]. Related somewhat to the Skyrme-Hartree-Fock model is the relativistic mean-field (RMF) approach [31,32], which also gives single-particle motion in a mean field, but as a solution to the Dirac equation as opposed to the Schrödinger equation. The RMF approach has some nice features such as the natural occurrence of the spin-orbit splitting without recourse to an assumed spin-orbit interaction.

The Hartree-Fock model alone is a purely single-particle model. That is to say, the many-body wave function is a single Slater determinant. This is a good approximation in closed-shell nuclei. Away from closed shells one usually needs to augment the ph mean field with a pairing interaction [33], which smears out the Fermi surface and breaks particle number symmetry. Observables with a classical analog, such as energy and shape, can be well reproduced in such mean field calculations. To obtain observables that are inherently quantum mechanical in nature, such as the discrete energy spectrum of excited states and transition probabilities, it is necessary to go beyond the mean field. One technique used is to restore the broken symmetries to obtain states with desired good quantum numbers. Restoration of the center-of-mass symmetry, broken in all mean field calculations, is a standard technique [34]. Particle number symmetry can be restored by projection techniques [35]. The restoration of angular momentum by projection has been shown to be important in the correct description of light nuclei in which shape coexistence occurs [36,37].

Another common approach to go beyond the mean field is to continue the perturbation expansion of which the HF approximation is equivalent to first order. Partial summation of higher order diagrams in the perturbation series can be carried out by means of the random phase approximation [38], which is particularly used to describe giant resonances but is applied also to residual interactions and ground state correlations [39].

While these methods of going beyond the mean field are all valid, we feel that it is desirable to be able to use normal perturbation theory to solve the MBSE. The HF approximation appears naturally in the hierarchy of perturbations and the ability to improve on the HF result, by using the same interaction that generates the mean field to complete the solution, has a desirable elegance and consistency.

We revisit the idea that it is possible to parametrize a nuclear interaction in such a way that it is weak enough with which to perform perturbation theory, thereby allowing correlated wave functions and observables to be calculated. Using the separable ansatz of previous weak interactions we have developed a density-dependent interaction, which we hope will provide some insight into the correlation structure of nuclear wave functions while retaining the quantitative power of contemporary effective interactions used in the Hartree-Fock method. In contrast to previous work with perturbative forces, the interaction is designed to be an effective interaction with parameters fitted to the properties of finite nuclei within the calculation framework for which it is intended.

The paper is organized as follows. In Sec. II we mention the relevant results from many-body perturbation theory used in this work. The separable interaction is given and discussed in Sec. III. Results of the calculation for doubly magic nuclei are summarized in Sec. IV. Derivation of the HF energy and potential is outlined in the Appendix.

II. MANY-BODY PERTURBATION CALCULATION

We calculate terms in the perturbation series for the energy to third order, using the Hartree-Fock solution as a starting point. The perturbation theory techniques are standard [40] and we state here the terms we calculate, namely, the one second-order contribution to the energy and the three third-order terms,

$$E_2=\frac{1}{4}\sum_{ab<\epsilon_F}\sum_{rs>\epsilon_F}\frac{|\langle ab|\tilde{V}|rs\rangle|^2}{\epsilon_a+\epsilon_b-\epsilon_r-\epsilon_s}, \tag{1}$$

$$E_3^{(pp)}=\frac{1}{8}\sum_{ab<\epsilon_F}\sum_{rs>\epsilon_F}\sum_{tu>\epsilon_F}\frac{\langle ab|\tilde{V}|rs\rangle\langle rs|\tilde{V}|tu\rangle\langle tu|\tilde{V}|ab\rangle}{(\epsilon_a+\epsilon_b-\epsilon_r-\epsilon_s)(\epsilon_a+\epsilon_b-\epsilon_t-\epsilon_u)}, \tag{2}$$

$$E_3^{(hh)}=\frac{1}{8}\sum_{ab<\epsilon_F}\sum_{cd<\epsilon_F}\sum_{rs>\epsilon_F}\frac{\langle ab|\tilde{V}|rs\rangle\langle cd|\tilde{V}|ab\rangle\langle rs|\tilde{V}|cd\rangle}{(\epsilon_a+\epsilon_b-\epsilon_r-\epsilon_s)(\epsilon_c+\epsilon_d-\epsilon_t-\epsilon_u)}, \tag{3}$$

$$E_3^{(ph)}=\sum_{abc<\epsilon_F}\sum_{rst>\epsilon_F}\frac{\langle ab|\tilde{V}|rs\rangle\langle cr|\tilde{V}|at\rangle\langle st|\tilde{V}|cb\rangle}{(\epsilon_a+\epsilon_b-\epsilon_r-\epsilon_s)(\epsilon_b+\epsilon_c-\epsilon_s-\epsilon_t)}, \tag{4}$$

in which the tildes over the potential indicate that the matrix element is antisymmetrized. The potential V is the two-body part of the Hamiltonian of the system. The state vectors label HF single-particle states, whose energies are given by the subscripted ϵ's.

In the present work, the Hartree-Fock problem is solved in a basis of spherical harmonic oscillator states. This yields, along with the hole states, a large number of particle states with which to directly evaluate the above sums. A sufficient number of states is used so that the positive energy particle states are oscillatory over the size of the nucleus and that both the HF solution and the perturbation corrections are reasonably converged.

It is important to note that our interaction is not intended to fit scattering data, having as it does, density dependence. On the level of the perturbation theory it is necessary to treat the density functions as just the spatial form of the interaction, rather than a representation of a many-body force. This is to be considered a part of the present model. To do otherwise would be to surrender the simplifications our weak, separable potential affords.

III. INTERACTION

We have developed an interaction written in the form of a sum of separable terms, which is to say it is in the form $V(r_1,r_2)\sim\Sigma g(r_1)g(r_2)$. The functions g carry no angular momentum ($l=0$), and the force is dubbed a monopole-monopole interaction. For future applications, it is intended to include higher multipole forces, with $l=1,2,\ldots$, within our framework as these will presumably be necessary for calculation of excited states and deformed nuclei. Although higher multipole forces will give contributions in spherical nuclei from the exchange term in Hartree-Fock order and via correlations in perturbation theory, they are not included in the present calculation since it seems unwise to attempt to fit the parameters of such forces to ground states of spherical nuclei alone.

In coordinate space, the monopole interaction is written as

$$\begin{aligned}V(\vec{r}_1,\vec{r}_2)=&W_a f_a \rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)\\&\times[1+a_a(t_1^+t_2^-+t_1^-t_2^+)+4b_a t_{1z}t_{2z}]\\&+W_r f_r \rho^{\beta_r}(\vec{r}_1)\rho^{\beta_r}(\vec{r}_2)\\&\times[1+a_r(t_1^+t_2^-+t_1^-t_2^+)+4b_r t_{1z}t_{2z}]\\&+k\nabla_1^2\rho(\vec{r}_1)\nabla_2^2\rho(\vec{r}_2),\end{aligned}\tag{5}$$

where the function f_ξ is defined as

$$f_\xi=\left[\int d\vec{r}\rho^{\alpha_\xi}(\vec{r})\right]^{-1}\tag{6}$$

for subscripts $\xi=a$ and $\xi=r$. The operators t^+, t^-, and t_z are isospin raising, lowering, and z axis projection operators, respectively. Throughout this work, the three terms in Eq. (5) are referred to, in the order in which they appear in the above expression, as the attractive, repulsive, and derivative terms.

In addition, the spin-orbit force is taken to be

$$V_{\text{s-o}}(\vec{r})=c\frac{1}{r}\frac{\partial\rho}{\partial r}\vec{l}\cdot\vec{s},\tag{7}$$

which is similar to that used in the modified delta interaction [24].

The parameters W_a, α_a, β_a, a_a, b_a, W_r, α_r, β_r, a_r, b_r, k, and c are to be fitted to experimental data.

One notices that the two-body interaction consists of a sum of terms, each of which is separable in form and that the expressions for the attractive and repulsive terms in Eq. (5) differ only by the values of their parameters.

The energy E_{pot} due to the interaction (5) in the Hartree-Fock approximation is derived in the Appendix [Eqs. (A2), (A3), and (A15)] and is presented here,

$$\begin{aligned}E_{HF}&=T+E_{\text{Coul}}+E_{\text{pot}}\\&=T+E_{\text{Coul}}+\sum_{\xi=a,r}\left\{\frac{1}{2}W_\xi f_\xi N_\xi^2-\frac{1}{2}W_\xi f_\xi M_\xi\right.\\&\quad\left.+\frac{1}{2}W_\xi b_\xi f_\xi(\Delta N_\xi)^2-\frac{1}{2}W_\xi f_\xi[b_\xi M_\xi+a_\xi M_\xi^{(\tau\bar{\tau})}]\right\}\\&\quad+\frac{1}{2}kN_d^2+cN_w,\end{aligned}\tag{8}$$

where T is the kinetic energy, E_{Coul} is the direct Coulomb energy plus exchange in the Slater approximation. The following quantities have been defined:

$$N_\xi=\int d\vec{r}\rho^{\beta_\xi+1}(\vec{r}),\tag{9}$$

$$\begin{aligned}M_\xi=\int\int d\vec{r}_1 d\vec{r}_2[&\rho_p(\vec{r}_1,\vec{r}_2)\rho^{\beta_\xi}(\vec{r}_1)\rho^{\beta_\xi}(\vec{r}_2)\rho_p(\vec{r}_1,\vec{r}_2)\\&+\rho_n(\vec{r}_1,\vec{r}_2)\rho^{\beta_\xi}(\vec{r}_1)\rho^{\beta_\xi}(\vec{r}_2)\rho_n(\vec{r}_1,\vec{r}_2)],\end{aligned}\tag{10}$$

$$\Delta N_\xi=\int d\vec{r}\rho^{\beta_\xi}(\vec{r})\delta\rho(\vec{r}),\tag{11}$$

$$\begin{aligned}M_\xi^{(\tau\bar{\tau})}=\int\int d\vec{r}_1 d\vec{r}_2[&\rho_p(\vec{r}_1,\vec{r}_2)\rho^{\beta_\xi}(\vec{r}_1)\rho^{\beta_\xi}(\vec{r}_2)\rho_n(\vec{r}_1,\vec{r}_2)\\&+\rho_n(\vec{r}_1,\vec{r}_2)\rho^{\beta_\xi}(\vec{r}_1)\rho^{\beta_\xi}(\vec{r}_2)\rho_p(\vec{r}_1,\vec{r}_2)],\end{aligned}\tag{12}$$

$$N_d=\int d\vec{r}\rho(\vec{r})\nabla^2\rho(\vec{r}),\tag{13}$$

$$N_w=\int d\vec{r}\frac{1}{r}\frac{\partial\rho}{\partial r}\rho_w(\vec{r}),\tag{14}$$

and the following densities are used:

$$\begin{aligned}\rho(\vec{r})&=\rho_p(\vec{r})+\rho_n(\vec{r})\\&=\sum_{i<\epsilon_F\in p}\varphi_i^*(\vec{r})\varphi_i(\vec{r})+\sum_{i<\epsilon_F\in n}\varphi_i^*(\vec{r})\varphi_i(\vec{r}),\end{aligned}\tag{15}$$

$$\rho(\vec{r}_1,\vec{r}_2)=\rho_p(\vec{r}_1,\vec{r}_2)+\rho_n(\vec{r}_1,\vec{r}_2)$$
$$=\sum_{i<\epsilon_F\in p}\varphi_i^*(\vec{r}_1)\varphi_i(\vec{r}_2)+\sum_{i<\epsilon_F\in n}\varphi_i^*(\vec{r}_1)\varphi_i(\vec{r}_2), \tag{16}$$

$$\delta\rho(\vec{r})=\rho_p(\vec{r})-\rho_n(\vec{r}), \tag{17}$$

$$\rho_w(\vec{r})=\sum_{i<\epsilon_F}\frac{1}{2}[j_i(j_i+1)-l_i(l_i+1)-3/4]\varphi_i^*(\vec{r})\varphi_i(\vec{r}). \tag{18}$$

The variation of the total energy is carried out in the Appendix [see Eqs. (A9), (A11), (A13), and (A18)]. The resulting local Hartree-Fock potential is

$$U_{L,\tau}(\vec{x})=\sum_{\xi=a,r}\{W_\xi f_\xi[N_\xi(\beta_\xi+1)+b_\xi\Delta_\tau N_\xi]\rho^{\beta_\xi}(\vec{x})$$
$$-W_\xi(\alpha_\xi/2)f_\xi^2[N_\xi^2+b_\xi(\Delta N_\xi)^2-(1+b_\xi)M_\xi$$
$$-a_\xi M_\xi^{(\tau\bar{\tau})}]\rho^{\alpha_\xi-1}(\vec{x})-W_\xi f_\xi\beta_\xi[(1+b_\xi)G_\xi(\vec{x})$$
$$+a_\xi G_\xi^{(\tau\bar{\tau})}(\vec{x})]\rho^{\beta_x-1}(\vec{x})+[W_\xi b_\xi\beta_\xi f_\xi\Delta N_\xi]$$
$$\times\rho^{\beta_x-1}(\vec{x})\delta\rho(\vec{x})\}+2kN_d\nabla^2\rho(\vec{x}), \tag{19}$$

which differs for protons ($\tau=p$) and neutrons ($\tau=n$) through the function

$$\Delta_\tau N_\xi=\begin{cases}\Delta N_\xi, & \tau=p\\ -\Delta N_\xi, & \tau=n.\end{cases} \tag{20}$$

The other newly introduced functions in Eq. (19) are

$$G_\xi(\vec{x})=G_\xi^{(pp)}(\vec{x})+G_\xi^{(nn)}(\vec{x})$$
$$=\int d\vec{r}[\rho_p(\vec{r},\vec{x})\rho^{\beta_\xi}(r)\rho_p(\vec{x},\vec{r})$$
$$+\rho_n(\vec{r},\vec{x})\rho^{\beta_\xi}(\vec{r})\rho_n(\vec{x},\vec{r})],$$
$$G_\xi^{(\tau\bar{\tau})}(\vec{x})=G_\xi^{(pn)}(\vec{x})+G_\xi^{(np)}(\vec{x})$$
$$=\int d\vec{r}[\rho_p(\vec{r},\vec{x})\rho^{\beta_\xi}(r)\rho_n(\vec{x},\vec{r})$$
$$+\rho_n(\vec{r},\vec{x})\rho^{\beta_\xi}(\vec{r})\rho_p(\vec{x},\vec{r})]. \tag{21}$$

In addition, the nonlocal component to the mean field is [see Eq. (A14)]

$$U_{NL,\tau}(\vec{x},\vec{x}')=\sum_{\xi=a,r}W_x f_x\rho^{\beta_\xi}(\vec{x})\rho^{\beta_\xi}(\vec{x}')\{(1+b_\xi)\rho_\tau(\vec{x},\vec{x}')$$
$$+a_\xi\rho_\tau^{-}(\vec{x},\vec{x}')\}, \tag{22}$$

and there is a state-dependent potential from the spin-orbit interaction of the form

$$U_{\rm so}(\vec{x})\varphi_i(\vec{x})=c\left(w_i\frac{1}{x}\frac{\partial\rho}{\partial x}-\frac{1}{x}\frac{\partial\rho_w}{\partial x}-\frac{1}{x^2}\rho_w(\vec{x})\right)\varphi_i(\vec{x}), \tag{23}$$

where $w_i=1/2[j_i(j_i+1)-l_i(l_i+1)-3/4]$ is the spin-orbit weight factor.

Note that the one-body spin-orbit term could be taken as either a one-body force, or as a one-body potential derived from a two-body force. Since the latter approach would render the perturbation calculation problematic due to the absence of a suitable form of the two-body force, we choose the former approach. Hence, since the force is density dependent, we have also included the rearrangement contribution to the HF potential. Only the nonrearrangement term actually gives rise to the spin-orbit splittings, but the rearrangement terms, coming as they do from a variational principle, result in a lowering of the HF energy. Combining the potentials (19), (22), and (23) gives us the HF equation

$$U_{L,\tau}(\vec{x})\varphi_i(\vec{x})+\int d\vec{x}'U_{NL,\tau}(\vec{x},\vec{x}')\varphi_i(\vec{x}')+U_{\rm so}(\vec{x})\varphi_i(\vec{x})$$
$$=\varepsilon_i\varphi_i(\vec{x}). \tag{24}$$

In this potential as well as in the expression for the total energy [Eq. (8)], the exchange contribution from the derivative term is omitted. While it would, in principle, be desirable to include this term, the calculational complexity involved in doing so has forced the omission in the present case. However, for the main attractive and repulsive terms, the exchange part is much smaller than the direct, and the direct derivative term gives a rather small contribution to the mean field and the binding energy in comparison to the other direct terms, so it is not considered an unwarranted approximation to neglect the effects of this term.

The interaction has some interesting or unusual characteristics. Its separability means that it does not satisfy Gallilean invariance. This choice was motivated by the desire to ensure that the force is perturbative and is justified by the results. Since our calculation is based upon a mean field, Gallilean invariance is bound to be broken anyway. It may be possible to adapt one of the standard techniques of symmetry restoration to our case [34], although a rigorous correction would destroy the mean field and would necessitate a reformulation of the perturbation calculation.

Also, we use an unusual form for the isospin exchange operator in which we stretch the more familiar $\tau_1\cdot\tau_2$ form to allow a different strength in the z direction in isospin space than in the x and y directions. This gives us extra degrees of freedom in fitting parameters to the data.

The choice of omitting a spin-spin ($\sigma_1\cdot\sigma_2$) type force yet having an isospin-isospin type force is motivated by the nuclei under study. All the closed-shell nuclei are spin saturated and would contribute only through the exchange term in the HF order. For this separable interaction, the space-exchange terms are rather small and a spin-spin force would add little to the results. In addition, even if the effects in closed-shell nuclei are important, it does not seem reasonable

to fit this term to closed-shell nuclei alone. It remains an open question whether such a force will prove necessary or useful in open-shell nuclei.

It is interesting to compare the leading terms in the HF mean field to that of other models. The first term of Eq. (19) gives us this as

$$U(\vec{x}) \sim \sum_{\xi=a,r} C_\xi (f_\xi N_\xi) \rho^{\beta_\xi}(\vec{x}), \tag{25}$$

where C_ξ is a combination of constants. The product $f_\xi N_\xi$ is

$$f_\xi N_\xi = \frac{\int d\vec{r} \rho^{\beta_\xi + 1}(\vec{r})}{\int d\vec{r} \rho^{\alpha_\xi}(\vec{r})}. \tag{26}$$

If $\beta_\xi + 1 = \alpha_\xi$ then the product $f_\xi N_\xi$ is unity and the leading mean-field terms go like

$$U(\vec{x}) \sim C_a \rho^{\beta_a}(\vec{x}) + C_r \rho^{\beta_r}(\vec{x}), \tag{27}$$

which for the special case $\beta_a = 1$, are the same as the terms in the Skyrme mean field proportional to the parameters t_0 and t_3, which give the bulk of the binding energy and saturation properties. In this work, we do not strictly keep $\beta_\xi + 1 = \alpha_\xi$, thus allowing for some A dependence of the coefficients in the mean-field potential. The fact that one can get similar results in a mean-field calculation from two very different interactions will be reflected in different results in the full perturbation series.

IV. DOUBLY (SEMI)MAGIC NUCLEI

In order to find the best set of parameters for the interaction (5), calculations have been made of 14 doubly closed-shell nuclei across the periodic table. They are ^{16}O, ^{34}Si, ^{40,48}Ca, ^{48,56,68,78}Ni, ^{90}Zr, ^{100,114,132}Sn, ^{146}Gd, and ^{208}Pb. The nuclei represent a selection of doubly closed (sub)shell nuclei both close to and far from stability. There is limited experimental information about ^{48}Ni [41] and ^{100}Sn [42]. The ability to reproduce the properties of such exotic nuclei will be important for the applications of our technique and discrepancies will help direct refinements.

A Hartree-Fock code assuming spherical symmetry and representing wave functions in a basis of spherical harmonic oscillator states was used to calculate uncorrelated wave functions. Perturbation corrections to the binding energy were directly evaluated using the results of the HF calculation. The results presented here were obtained in a basis of 12 expansion coefficients per single-particle wave function and iterated until the HF energy had converged to within 1 keV. The parameters of the force were fitted to binding energies to second order and charge radii, charge density distributions, single-particle energies and spin-orbit splittings to HF order of the nuclei listed above where experimental data were available and are presented in Table I.

The results of the calculated energies, in HF order and in each order of perturbation theory are presented in Table II.

TABLE I. Monopole force parameters.

W_a	α_a	β_a	a_a	b_a
-1543.8 MeV fm^3	2.0	1.0	-0.4295	-0.4448
W_r	α_r	β_r	a_r	b_r
1778.0 MeV fm$^{3.8265}$	2.2165	1.246	-1.4788	-0.3146
c			k	
160.0 MeV fm^5			16.0 MeV fm^{10}	

The differences between the HF energy (8), $E_{\rm cal} = E_{\rm HF}$ and the experimental ground state energy $E_{\rm exp}$ and between HF and second order perturbation correction (1), $E_{\rm cal} = E_{\rm HF} + E_2$ and experiment are shown in Fig. 1. The experimental energies are taken from the mass table of Audi and Wapstra [43] with two exceptions—an estimate of the mass of the recently observed nucleus ^{48}Ni [44] and the measured mass of ^{100}Sn [45]. The energy for ^{78}Ni was taken from [43] in which extrapolated values are given, which are thought to be in error by less than 0.2%.

One sees from Fig. 1 that most of the nuclei fit the binding energy to within $\sim 2\%$. The most obvious exception is ^{16}O, which is quite underbound. This may be due to the omission of a center-of-mass correction. It was not calculated in this case as discussed in Sec. III. We also mention that the correlation energy, as we shall shortly see, is greater per particle in the lightest nuclei, so correlations from higher multipole forces may play a significant role in correcting this discrepancy.

A general trend can be seen in which lighter nuclei are somewhat overbound and the heaviest are underbound. It is the exceptions that conspire to stop the fitting algorithm from doing better, but the somewhat systematic nature of this discrepancy suggests that a better mass or isospin dependence may improve matters. It is unclear as yet the extent to which multipole correlations or a spin-spin force would improve the fit to spherical nuclei. That question awaits the study of deformed nuclei and excited states.

In Table III a comparison is made of the quality of the fit to the binding energy to properties of the same nuclei calculated with a selection of Skyrme parametrizations. The parametrizations used are SIII [46], SkP [29], SLy4 [47], and SkI4 [30]. In this comparison, it is seen that the energies from the different Skyrme parametrizations are of a similar quality, all reproducing the binding energies of closed-shell nuclei very well, with only a few binding energies being reproduced no better than 1%—including ^{48}Ni whose experimental value is in any case not well known. It is clear that the results from the separable force are somewhat worse. Particularly problematic is ^{16}O, whose large underbinding was mentioned above, and also ^{48}Ni, which is as with the Skyrme parametrizations, overbound although more so with the separable interaction.

Results for one-body properties in HF order are also presented. Comparison of the rms radii to experiment [48] and to the selection of Skyrme interactions is made in Table IV. One-body observables are generally reproduced better in the

TABLE II. Hartree-Fock energy (8) and corrections from perturbation theory (1)–(4) compared with experimental values from [43]. All energies are in MeV.

Nucleus	E_{HF}	$E^{(2)}$	$E^{(3)_{hh}}$	$E^{(3)_{pp}}$	$E^{(3)_{ph}}$	E_{HF+2+3}	κ	Expt.
^{16}O	−109.32	−3.31	−0.1365	−0.3624	+0.921	−112.21	0.063	−127.68
^{34}Si	−280.88	−7.37	−0.0384	−0.4830	+1.223	−287.55	0.232	−283.43
^{40}Ca	−334.53	−2.51	−0.0323	−0.1114	+0.233	−336.95	0.052	−342.00
^{48}Ca	−417.01	−5.97	−0.0189	−0.2725	+0.273	−422.70	0.202	−416.16
^{48}Ni	−360.69	−6.57	−0.0130	−0.2058	+0.427	−367.05	0.234	−348.33
^{56}Ni	−481.25	−2.31	−0.0210	−0.0643	+0.123	−483.52	0.046	−483.99
^{68}Ni	−593.33	−6.00	−0.0109	−0.2091	+0.484	−598.85	0.221	−590.43
^{78}Ni	−651.90	−8.34	−0.0053	−0.1458	+0.477	−659.92	0.342	−641.38
^{90}Zr	−782.70	−3.91	−0.0070	−0.1257	+0.103	−786.51	0.149	−783.89
^{100}Sn	−825.65	−1.71	−0.0060	−0.0220	+0.048	−827.35	0.039	−826.81
^{114}Sn	−963.20	−4.04	−0.0046	−0.1093	+0.226	−967.12	0.162	−971.57
^{132}Sn	−1097.65	−6.17	−0.0023	−0.0864	+0.209	−1103.70	0.287	−1102.92
^{146}Gd	−1190.32	−3.42	−0.0026	−0.0699	+0.142	−1193.66	0.146	−1204.44
^{208}Pb	−1599.04	−4.51	−0.0013	−0.0664	+0.108	−1603.51	0.233	−1636.45

HF calculation alone than the binding energies. The comparison of the calculated charge radii with experiment is generally more favorable than the energy data. The radius of oxygen is too large by about 5%, which is consistent with its underbinding. It can be seen that the agreement with experiment is of the same level as the Skyrme interactions. Perturbative corrections to the one-body observables such as the densities, and hence radii, will be calculated in future work.

Figures 2 and 3 show the calculated electron scattering form factors for a representative light nucleus, ^{40}Ca, and a heavy one, ^{208}Pb, compared to experiment [48]. The proton density from the HF calculation was corrected for the finite proton size by folding with a Gaussian to give the charge density, from which the radii and form factors were calculated. The form factors agree with experiment rather well, which is expected given the generally correct radii.

Single-particle energies are shown in Figs. 4 and 5 for ^{40}Ca and ^{208}Pb, respectively. The single-particle energies of a density-dependent Hartree-Fock calculation do not directly correspond to an experimental observable, so caution should be used in comparing values. It can be seen that the level spacings and shell closures are better reproduced in ^{208}Pb, which is true of heavy nuclei in general. The comparatively poorer results in light nuclei seem to be common to mean-field approaches [49].

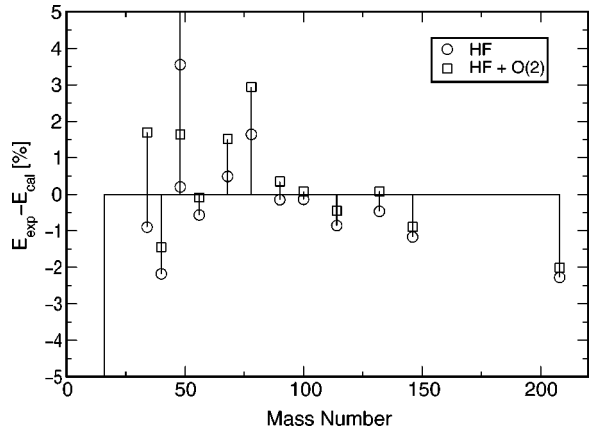

FIG. 1. Deviation of Hartree-Fock energy from experiment. Negative errors denote underbinding. Note that ^{16}O and the second order result for ^{48}Ni are beyond the scale.

Table V shows spin-orbit splittings for some cases where the experimental values are known. The ''experimental'' data presented represent that used in previous work for fitting effective interactions to data [47,50,51]. Clearly the splittings are all systematically small. This could be remedied by an increase in the spin-orbit coefficient c. In a previous work [52], a value 10% higher than ours was used for the same spin-orbit interaction and hence the spin-orbit splittings were more realistic. The lower value used in our work is the result of a compromise between the reproduction of the spin-orbit splittings and the total binding energies. This is an indication that a more suitable spin-orbit potential needs to be sought.

TABLE III. Percentage error in binding energy. Negative values are underbound. Separable force is HF+perturbations, Skyrme calculations are HF+pairing.

Nucleus	Sep.	SIII	SkP	SLy4	SkI4
^{16}O	−12.10	0.36	−0.12	0.19	0.57
^{34}Si	1.45	0.43	0.92	1.08	1.06
^{40}Ca	−1.49	−0.18	0.21	0.50	0.51
^{48}Ca	1.61	0.40	−0.04	−0.63	0.31
^{48}Ni	5.37	1.52	1.22	0.74	1.58
^{56}Ni	−0.10	−0.22	−1.11	0.09	−0.29
^{68}Ni	1.43	−0.25	0.09	0.81	0.26
^{78}Ni	2.89	0.58	−0.05	−0.29	0.21
^{90}Zr	0.33	−0.14	−0.14	−0.11	0.13
^{100}Sn	0.07	0.14	−0.51	0.75	0.28
^{114}Sn	−0.46	−0.71	−0.48	0.09	−0.56
^{132}Sn	0.07	0.10	−0.31	0.14	−0.12
^{146}Gd	−0.90	−0.33	−0.41	−0.20	−0.24
^{208}Pb	−2.01	−0.17	−0.27	0.21	−0.24

TABLE IV. Comparison of charge radii between experiment, the separable interaction, and a selection of Skyrme interactions. The model-dependent experimental values are from [48].

Nucleus	Exp.	Sep.	SIII	SkP	SLy4	SkI4
^{16}O	2.69	2.85	2.71	2.80	2.76	2.72
^{34}Si		3.19	3.23	3.25	3.23	3.21
^{40}Ca	3.48	3.54	3.48	3.52	3.49	3.45
^{48}Ca	3.48	3.47	3.52	3.53	3.51	3.45
^{48}Ni		3.88	3.77	3.82	3.79	3.80
^{56}Ni	3.78	3.84	3.80	3.80	3.78	3.74
^{68}Ni		3.89	3.94	3.93	3.91	3.81
^{78}Ni		3.87	4.02	3.99	3.98	3.97
^{90}Zr	4.27	4.29	4.31	4.30	4.28	4.23
^{100}Sn		4.60	4.53	4.52	4.50	4.45
^{114}Sn	4.60	4.65	4.66	4.62	4.62	4.59
^{132}Sn		4.66	4.78	4.74	4.73	4.70
^{146}Gd	4.96	5.02	5.03	5.00	4.99	4.94
^{208}Pb	5.50	5.50	5.57	5.52	5.51	5.48

The perturbation corrections to the energy are seen to be rather small in all nuclei considered. This is consistent with our goal that the mean-field solution should be close to the exact solution of the MBSE. The size of the second order correlation is roughly constant across the periodic table. It is characterized by a dimensionless strength parameter κ defined as

$$\kappa=\frac{1}{4}\sum_{ab\leqslant\epsilon_F}\sum_{rs>\epsilon_F}\frac{\langle ab|\tilde{V}|rs\rangle\langle rs|\tilde{V}|ab\rangle}{(\epsilon_a+\epsilon_b-\epsilon_r-\epsilon_s)^2}, \tag{28}$$

which is related to the *wound integral* [53] and is proportional to the number of $2p2h$ states excited due to the second order perturbation.

Figure 6 shows the correlation structure from the second order correction in the $N=Z$ nucleus ^{40}Ca and the nuclei ^{48}Ca and ^{208}Pb. The contribution to the second order energy is defined as a function of one of the particle states r,

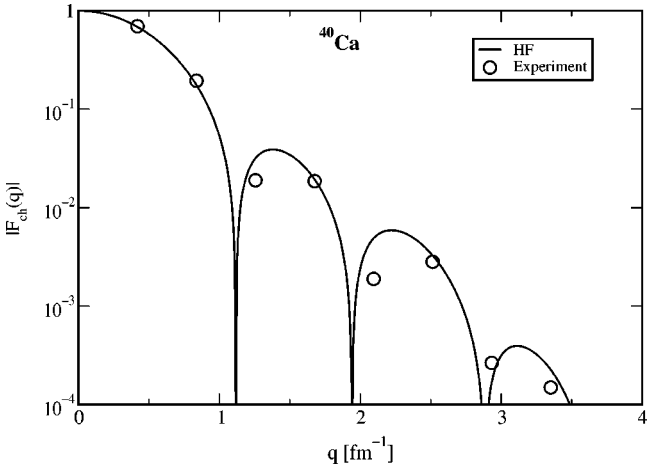

FIG. 2. Charge form factor in ^{40}Ca.

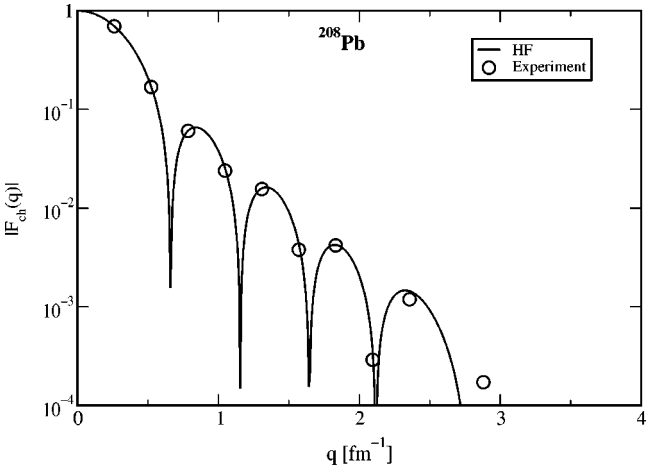

FIG. 3. Charge form factor in ^{208}Pb.

$$E_2(|r\rangle)=\frac{1}{4}\sum_{ab\leqslant\epsilon_F}\sum_{s>\epsilon_F}\frac{|\langle ab|\tilde{V}|rs\rangle|^2}{\epsilon_a+\epsilon_b-\epsilon_r-\epsilon_s}. \tag{29}$$

The plot shows the contribution to the total second order energy correction as a function of the single particle energy ϵ_r in 5-MeV wide bins. In all three cases particles are dominantly excited to low-lying states above the Fermi level. This results in a ground state with occupation probabilities similar to those that result from pairing forces. It is also a further indication that perturbation theory makes sense for our interaction since it does not predict excitation of particles in the ground state to extremely high energies.

Since the calculations were made using only a monopole force, the correlation structure is not expected to be complete. Only corrections involving simultaneous $l=0$ scattering of two particles is included. An indication of this incompleteness is seen in the difference between the results for $N=Z$ and $N\neq Z$ nuclei. The second order correction in ^{48}Ca is much larger than that in ^{40}Ca, due to the possibility of an $f_{7/2}$ neutron exciting to the $f_{7/2}$ proton state while another proton excites to a neutron state. This extra excitation is the labeled peak in Fig. 6. As well as having large wave function overlaps, the energy denominator in this case is smaller than in

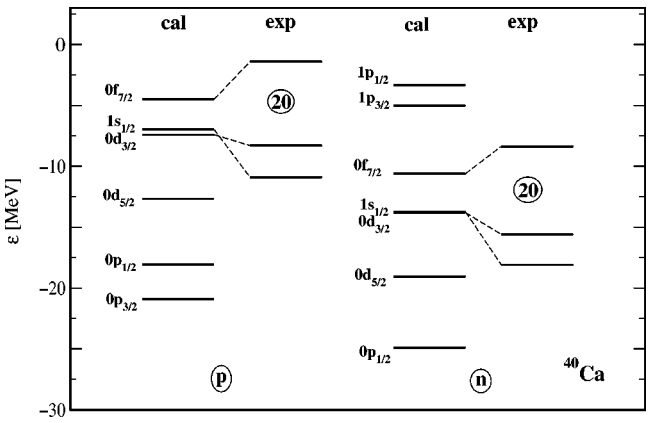

FIG. 4. Single-particle energies in ^{40}Ca compared to experiment [49].

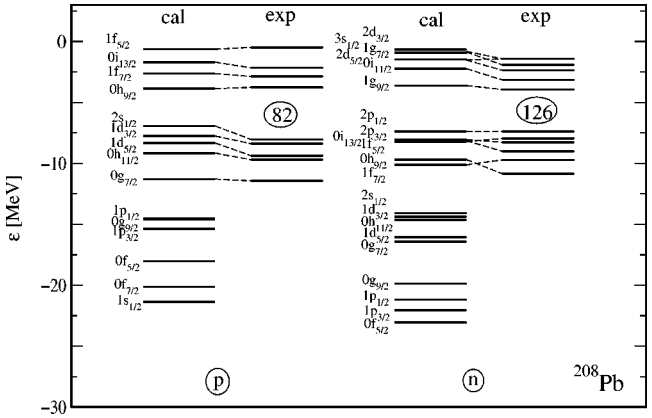

FIG. 5. Single-particle energies in ^{208}Pb compared to experiment [49].

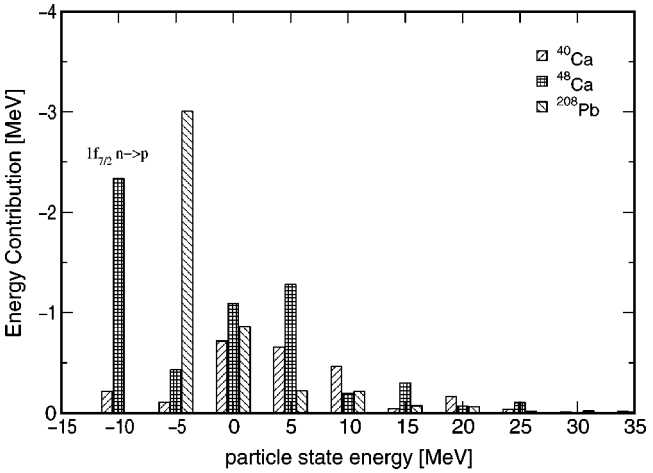

FIG. 6. Second order ground state correlation structure in ^{40}Ca, ^{48}Ca, and ^{208}Pb.

any other possible monopole excitation, which must excite any particle across major shells to keep all angular and isospin quantum numbers the same. When general excitations are permitted by higher multipole forces $l=1,2,\ldots$, this difference between correlations in $N=Z$ and $N\neq Z$ nuclei will be smoothed out. For this reason, the correlation energies should not be considered too quantitatively at this stage but rather as an indication of the perturbative properties of the interaction.

Comparing the form of our interaction to that of Skyrme's suggests other possible sources of improvement to the model. One such may come from a better parametrization of the spin-orbit interaction. A two-body form that fits the philosophy of the separable effective interaction has not been found, but may be necessary to give the correct contribution to the binding energy and provide the best isospin dependence. It may also prove fruitful to explore a more general term, dependent upon the derivatives of the density, than our single term with parameter k, as is found in the Skyrme interaction, which has two terms with parameters t_1 and t_2 that often carry further exchange parameters x_1 and x_2.

V. CONCLUSION

We have presented a new effective nuclear interaction that is designed for use in calculations that go beyond the mean field. The technique of using perturbation theory to build correlations on top of the Hartree-Fock result is applicable to our interaction and results in small corrections to the single-particle behavior. A monopole-monopole force alone gives reasonable results for the ground state properties of spherical doubly magic nuclei. It is expected that the addition of multipole forces will improve these results, particularly through the completion of the correlation structure. Such multipole forces will also presumably be important in giving the correct shapes of deformed nuclei, which are the subject of a forthcoming study, and the correct description of excited states.

TABLE V. Spin-orbit splittings in HF calculation. For source of experimental values, see text.

Levels	Splitting (HF)	Splitting (exp)
^{16}O, $0p(p)$	4.2	6.3
^{16}O, $0p(n)$	4.3	6.1
^{40}Ca, $0d(p)$	5.3	7.2
^{40}Ca, $0d(n)$	5.3	6.3
^{208}Pb, $2p(n)$	0.67	0.89

ACKNOWLEDGMENTS

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APPENDIX: HF ENERGY AND POTENTIAL

The interaction V is given in Eq. (5). Its expectation value is the contribution it makes to the total energy and is

$$E_{\rm pot}=\frac{1}{2}\sum_{ij<\epsilon_F}\langle ij|V\{|ij\rangle-|ji\rangle\}. \tag{A1}$$

If we consider just the *attractive* term—that is, the term whose parameters have the subscript a—then we will obtain the contribution from the repulsive term by simply substituting the subscript a by r:

$$\begin{aligned}E_a=&\frac{1}{2}W_a f_a\sum_{ij<\epsilon_F}\langle ij|\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)\{|ij\rangle-|ji\rangle\}\\&+\frac{1}{2}W_a f_a a_a\sum_{ij<\epsilon_F}\langle ij|\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)(t_1^+t_2^-+t_1^-t_2^+)\\&\times\{|ij\rangle-|ji\rangle\}+\frac{1}{2}W_a f_a b_a\\&\times\sum_{ij<\epsilon_F}\langle ij|\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)4t_{1z}t_{2z}\{|ij\rangle-|ji\rangle\}.\end{aligned} \tag{A2}$$

Taking the first line, the matrix element is represented in space (and spin and isospin) coordinates,

$$\begin{aligned}
&\frac{1}{2}W_a f_a \sum_{ij<\epsilon_F} \int d\vec{r}_1 \int d\vec{r}_2 \phi_i^*(\vec{r}_1)\phi_j^*(\vec{r}_2)\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)\phi_i(\vec{r}_1)\phi_j(\vec{r}_2) \\
&\quad -\frac{1}{2}W_a f_a \sum_{ij<\epsilon_F} \int d\vec{r}_1 \int d\vec{r}_2 \phi_i^*(\vec{r}_1)\phi_j^*(\vec{r}_2)\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)\phi_j(\vec{r}_1)\phi_i(\vec{r}_2) \\
&= \frac{1}{2}W_a f_a \int d\vec{r}_1 \rho^{\beta_a+1}(\vec{r}_1) \int d\vec{r}_2 \rho^{\beta_a+1}(\vec{r}_2) - \frac{1}{2}W_a f_a \int d\vec{r}_1 \int d\vec{r}_2 \rho_p(\vec{r}_1,\vec{r}_2)\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)\rho_p(\vec{r}_2,\vec{r}_1) \\
&\quad -\frac{1}{2}W_a f_a \int d\vec{r}_1 \int d\vec{r}_2, \rho_n(\vec{r}_1,\vec{r}_2)\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)\rho_n(\vec{r}_2,\vec{r}_1) \\
&= \frac{1}{2}W_a f_a N_a^2 - \frac{1}{2}W_a f_a M_a ,
\end{aligned} \tag{A3}$$

where quantities defined in Sec. III are used. Note that integrals include sums over spinors and isospinors where appropriate, and the coordinates include spin and isospin coordinates where appropriate. Where densities are used instead of wave functions, the summing over isospin states has already been done and where densities do not carry isospin labels, the isoscalar density is assumed. See Eqs. (15) and (16) for definitions.

The second term in Eq. (A2) contains isospin-flipping operators whose action is to turn an isospin state where particle 1 is a proton and particle 2 a neutron, $|pn\rangle$, into $|np\rangle$ and vice versa. The direct contribution, in which the labels in the bra and the ket are in the same order is zero since all proton states are orthogonal to all neutron states. The exchange term is similar to that in Eq. (A3) but with a different isospin combination of the density matrices,

$$\begin{aligned}
&-\frac{1}{2}W_a f_a a_a \int d\vec{r}_1 \int d\vec{r}_2 \rho_p(\vec{r}_1,\vec{r}_2)\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)\rho_n(\vec{r}_2,\vec{r}_1) - \frac{1}{2}W_a f_a a_a \int d\vec{r}_1 \int d\vec{r}_2 \rho_n(\vec{r}_1,\vec{r}_2)\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)\rho_p(\vec{r}_2,\vec{r}_1) \\
&\quad = -\frac{1}{2}W_a f_a a_a M_a^{(\overline{\tau\tau})} .
\end{aligned} \tag{A4}$$

The third line of Eq. (A2) contains isospin-projection operators that have a value $+1/2$ when i and j are like particles and $-1/2$ when they are unlike. In the direct term this gives an energy of

$$\begin{aligned}
&\frac{1}{2}W_a f_a b_a \int d\vec{r}_1 \rho_p(\vec{r}_1)\rho^{\beta_a}(\vec{r}_1) \int d\vec{r}_2 \rho_p(\vec{r}_2)\rho^{\beta_a}(\vec{r}_2) + \frac{1}{2}W_a f_a b_a \int d\vec{r}_1 \rho_n(\vec{r}_1)\rho^{\beta_a}(\vec{r}_1) \int d\vec{r}_2 \rho_n(\vec{r}_2)\rho^{\beta_a}(\vec{r}_2) \\
&\quad -\frac{1}{2}W_a f_a b_a \int d\vec{r}_1 \rho_p(\vec{r}_1)\rho^{\beta_a}(\vec{r}_1) \int d\vec{r}_2 \rho_n(\vec{r}_2)\rho^{\beta_a}(\vec{r}_2) - \frac{1}{2}W_a f_a b_a \int d\vec{r}_1 \rho_n(\vec{r}_1)\rho^{\beta_a}(\vec{r}_1) \int d\vec{r}_2 \rho_p(\vec{r}_2)\rho^{\beta_a}(\vec{r}_2) \\
&= \frac{1}{2}W_a f_a b_a \left[\int d\vec{r}\rho_p(\vec{r})\rho^{\beta_a}(\vec{r}) \right]^2 + \frac{1}{2}W_a f_a b_a \left[\int d\vec{r}\rho_n(\vec{r})\rho^{\beta_a}(\vec{r}) \right]^2 - W_a f_a b_a \int d\vec{r}_1 \rho_n(\vec{r}_1)\rho^{\beta_a}(\vec{r}_1) \int d\vec{r}_2 \rho_p(\vec{r}_2)\rho^{\beta_a}(\vec{r}_2) \\
&= \frac{1}{2}W_a f_a b_a \left[\int d\vec{r}\{\rho_p(\vec{r}) - \rho_n(\vec{r})\}\rho^{\beta_a}(\vec{r}) \right]^2 \\
&= \frac{1}{2}W_a f_a b_a (\Delta N_a)^2 .
\end{aligned} \tag{A5}$$

The exchange term gives a contribution only when i and j have the same isospin quantum number, which is just like the case for having no isospin operator there so that the contribution is like that in Eq. (A3),

$$-\frac{1}{2}W_a f_a b_a M_a . \tag{A6}$$

The HF mean field is obtained by varying the total energy with respect to the single-particle states. This gives, for the case of the attractive term, without the explicit isospin dependence,

$$\frac{\delta}{\delta\phi_b(\vec{x})}\left(\frac{1}{2}W_a f_a N_a^2-\frac{1}{2}W_a f_a M_a\right)$$

$$=\frac{1}{2}W_a\frac{\delta f_a}{\delta\phi_b^*(\vec{x})}N_a^2+W_a f_a N_a\frac{\delta N_a}{\delta\phi_b^*(\vec{x})}$$

$$-\frac{1}{2}W_a\frac{\delta f_a}{\delta\phi_b^*(\vec{x})}M_a-\frac{1}{2}W_a f_a\frac{\delta M_a}{\delta\phi_b^*(\vec{x})}. \tag{A7}$$

The variation of the function f_a is given by

$$\frac{\delta f_a}{\delta\phi_b^*(\vec{x})}=\frac{\delta}{\delta\phi_b^*(\vec{x})}\left[\int\rho^{\alpha_a}(\vec{r})d\vec{r}\right]^{-1}$$

$$=-f_a^2\int d\vec{r}\frac{\delta\rho^{\alpha_a}(\vec{r})}{\delta\phi_b^*(\vec{x})}$$

$$=-f_a^2\alpha_a\int d\vec{r}\rho^{\alpha_a-1}(\vec{r})\frac{\delta\rho(\vec{r})}{\delta\phi_b^*(\vec{x})}$$

$$=-f_a^2\alpha_a\rho^{\alpha_a-1}(\vec{x})\phi_b(\vec{x}), \tag{A8}$$

so that the contributions of the two terms in Eq. (A7) involving the variation of f_a give a contribution to the HF mean field of

$$-W_a(\alpha_a/2)f_a^2(N_a^2-M_a)\rho^{\alpha_a-1}(\vec{x}). \tag{A9}$$

The function N_a is similar in form to f_a and the functional variation proceeds in a similar manner,

$$\frac{\delta N_a}{\delta\phi_b^*(\vec{x})}=\frac{\delta}{\delta\phi_b^*(\vec{x})}\int d\vec{r}\rho^{\beta_a+1}(\vec{r})=(\beta_a-1)\rho^{\beta_a}(\vec{x})\phi_b(\vec{x}) \tag{A10}$$

and the contribution from the second term in Eq. (A7) to the mean field is

$$W_a f_a N_a(\beta_a-1)\rho^{\beta_a}(\vec{x}). \tag{A11}$$

Finally, the functional variation of the exchange matrix element M_a is

$$\frac{\delta M_a}{\delta\phi_b^*(\vec{x})}=\frac{\delta}{\delta\phi_b^*(\vec{x})}\left(\sum_{ij<\epsilon_F}\int\int d\vec{r}_1 d\vec{r}_2\phi_i^*(\vec{r}_1)\phi_j^*(\vec{r}_2)\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)\phi_j(\vec{r}_1)\phi_i(\vec{r}_2)\right)$$

$$=2\sum_{ij<\epsilon_F}\int\int d\vec{r}_1 d\vec{r}_2\frac{\delta\phi_i^*}{\delta\phi_b^*(\vec{x})}\phi_j(\vec{r}_2)\rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)\phi_j(\vec{r}_1)\phi_i(\vec{r}_2)$$

$$+2\sum_{ij<\epsilon_F}\int\int d\vec{r}_1 d\vec{r}_2\phi_i^*(\vec{r}_1)\phi_j^*(\vec{r}_2)\frac{\delta\rho^{\beta_a}(\vec{r}_1)}{\delta\phi_b^*(\vec{x})}\rho^{\beta_a}(\vec{r}_2)\phi_j(\vec{r}_1)\phi_i(\vec{r}_2)$$

$$=2\sum_{j<\epsilon_F}\int d\vec{r}_2\phi_j^*(\vec{r}_2)\rho^{\beta_a}(\vec{x})\rho^{\beta_a}(\vec{r}_2)\phi_j(\vec{x})\phi_b(\vec{r}_2)$$

$$+2\sum_{ij<\epsilon_F}\int d\vec{r}_2\phi_i^*(\vec{x})\phi_j(\vec{r}_2)\beta_a\rho^{\beta_a-1}(\vec{x})\phi_b(\vec{x})\rho^{\beta_a}(\vec{r}_2)\phi_j(\vec{x})\phi_i(\vec{r}_2), \tag{A12}$$

where use is made of the symmetry of the integral to combine the four terms into two. The last term in Eq. (A12) gives rise to a local term in the mean field of

$$-W_a f_a\beta_a\sum_{i<\epsilon_F}\left[\int d\vec{r}\rho(\vec{r},\vec{x})\rho^{\beta_a}(\vec{r})\rho(\vec{x},\vec{r})\right]\rho^{\beta_a-1}(\vec{x})$$

$$=-W_a f_a\beta_a G_a(\vec{x})\rho^{\beta_a-1}(\vec{x}), \tag{A13}$$

where $G_a(\vec{x})$ has been defined as in Eq. (21).

The other term in Eq. (A12) gives rise to a truly nonlocal Fock term in the mean field,

$$U(\vec{x},\vec{x}')\phi_b(\vec{x})=-W_a f_a\sum_{i<\epsilon_F}\rho^{\beta_a}(\vec{x})\phi_i(\vec{x})$$

$$\times\left[\int d\vec{r}\phi_i^*(\vec{r})\rho^{\beta_a}(\vec{r})\phi_b(\vec{r})\right]. \tag{A14}$$

This completes the non-isospin-dependent part of the attractive force, and so also the repulsive part by change of subscript. The isospin-dependent terms are obtained in an

analogous way, except that when the variation applies to the density of a single nucleon species, the contribution to the mean field applies only to that species.

For the final term in Eq. (5), the so-called *derivative* term, only the direct part of the energy is at present considered. It is

$$E_{\mathrm{deriv}}=\frac{1}{2}k\sum_{ij<\epsilon_F}\langle ij|\nabla_1^2\rho(\vec{r}_1)\nabla_2^2(\vec{r}_2)|ij\rangle$$

$$=\frac{1}{2}k\int d\vec{r}_1\rho(\vec{r}_1)\nabla_1^2\rho(\vec{r}_1)\int d\vec{r}_2\rho(\vec{r}_2)\nabla_2^2\rho(\vec{r}_2)$$

$$=\frac{1}{2}kN_d^2. \tag{A15}$$

The functional variation proceeds as

$$\frac{\delta E_{\mathrm{deriv}}}{\delta\phi_b^*(\vec{x})}=kN_d\frac{\delta}{\delta\phi_b^*(\vec{x})}\int d\vec{r}\rho(\vec{r})\nabla^2\rho(\vec{r})$$

$$=kN_d\int d\vec{r}\left\{\frac{\delta\rho(\vec{r})}{\delta\phi_b^*(\vec{x})}\right\}\nabla^2\rho(\vec{r})+kN_d\int d\vec{r}\rho(\vec{r})$$

$$\times\left\{\frac{\delta}{\delta\phi_b^*(\vec{x})}\nabla^2\rho(\vec{r})\right\}. \tag{A16}$$

The first term gives a contribution to the mean field of

$$kN_d\nabla^2\rho(\vec{x}). \tag{A17}$$

By integrating the second term by parts twice, one in fact gets exactly the same contribution to the mean field again, so that the total contribution to the mean field from the direct term of the derivative interaction is

$$2kN_d\nabla^2\rho(\vec{r}). \tag{A18}$$

The exchange part of this term is not calculated.

[1] R. Machleidt, K. Holinde, and Ch. Elster, Phys. Rep. **149**, 1 (1987).
[2] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).
[3] J. Carlson, V. R. Pandharipande, R. B. Wiringa, Nucl. Phys. **A401**, 59 (1983).
[4] V. G. J. Stoks, R. A. M. Klomp, C. P. F. Terheggen, and J. J. de Swart, Phys. Rev. C **49**, 2950 (1994).
[5] V. I. Kukulin, V. N. Pomerantsev, and Amand Faessler, Phys. Rev. C **59**, 3021 (1999).
[6] R. B. Wiringa, Phys. Rev. C **43**, 1585 (1991).
[7] B. S. Pudliner, V. R. Pandharipande, and J. Carlson, Phys. Rev. C **56**, 1720 (1997).
[8] F. Coester, Nucl. Phys. **7**, 421 (1958).
[9] B. Mihaila and J. Heisenberg, Phys. Rev. C **59**, 1440 (1999).
[10] A. Fabrocini, F. Arias de Saavedra, G. Co', and P. Folgarait, Phys. Rev. C **57**, 1668 (1998).
[11] D. C. Zheng, B. R. Barrett, J. P. Vary, W. C. Haxton, and C.-L. Song, Phys. Rev. C **52**, 2488 (1995).
[12] L. Coraggio, A. Covello, A. Gargano, N. Itaco, and T. T. S. Kuo, Phys. Rev. C **58**, 3346 (1998).
[13] R. B. Wiringa, Steven C. Pieper, J. Carlson, and V. R. Pandharipande, Phys. Rev. C **62**, 014001 (2000).
[14] A. Kerman, Cargese Lect. Phys. **3**, 396 (1969).
[15] C. N. Bressel, A. K. Kerman, and B. Rouben, Nucl. Phys. **A124**, 624 (1969).
[16] B. Rouben, Ph.D. thesis, MIT, 1969.
[17] J. Zipse, Ph.D. thesis, MIT, 1970.
[18] E. Riihimäki, Ph.D. thesis, MIT, 1970.
[19] H. A. Bethe, Annu. Rev. Nucl. Sci. **21**, 93 (1971).
[20] D. R. Bés and Z. Szymanski, Nucl. Phys. **28**, 42 (1961).
[21] M. Baranger and K. Kumar, Nucl. Phys. **62**, 113 (1965).
[22] R. Devi and S. K. Khosa, Phys. Rev. C **54**, 1661 (1996).
[23] N. H. Kwong and H. S. Köhler, Phys. Rev. C **55**, 1650 (1997).
[24] J. W. Ehlers and S. A. Moszkowski, Phys. Rev. C **6**, 217 (1972).
[25] T. H. R. Skyrme, Philos. Mag. **1**, 1043 (1956).
[26] D. Vautherin and D. M. Brink, Phys. Rev. C **5**, 626 (1972).
[27] J. Decharge and D. Gogny, Phys. Rev. C **21**, 1568 (1980).
[28] P. Quentin and H. Flocard, Annu. Rev. Nucl. Sci. **28**, 523 (1978).
[29] J. Dobaczewski, H. Flocard, and J. Treiner, Nucl. Phys. **A422**, 103 (1984).
[30] P.-G. Reinhard and H. Flocard, Nucl. Phys. **A584**, 467 (1995).
[31] B. D. Serot and J. D. Walecka, Adv. Nucl. Phys. **16**, 1 (1986).
[32] P.-G. Reinhard, Rep. Prog. Phys. **52**, 439 (1989).
[33] P. Moller and J. R. Nix, Nucl. Phys. **A536**, 20 (1992).
[34] M. Bender, K. Rutz, P.-G. Reinhard, and J. A. Maruhn, Eur. Phys. J. A **7**, 467 (2000).
[35] D. Almehed, F. Dönau, S. Frauendorf, and R. G. Nazmitdinov, Phys. Scr. **T88**, 62 (2000).
[36] P.-H. Heenen, P. Bonche, S. Ćwiok, W. Nazerewicz, and A. Valor, RIKEN Rev. **10**, 1 (1999).
[37] R. Rodríguez-Guzmán, J. L. Egido, and L. M. Robledo, Phys. Lett. B **474**, 15 (2000).
[38] D. Bohm and D. Pines, Phys. Rev. **92**, 609 (1953).
[39] G. Bertsch and K. Hagino, nucl-th/0006032.
[40] J. Goldstone, Proc. R. Soc. London, Ser. A **239**, 267 (1957).
[41] B. Blank *et al.*, Phys. Rev. Lett. **84**, 1116 (2000).
[42] R. Schneider, Phys. Scr. **T56**, 67 (1995).
[43] G. Audi and A. H. Wapstra, Nucl. Phys. **A584**, 221 (1995).
[44] B. Alex Brown, Phys. Rev. C **43**, R1513 (1991).
[45] M. Chartier *et al.*, Phys. Rev. Lett. **77**, 2400 (1996).
[46] M. Beiner, H. Flocard, N. Van Giai, and P. Quentin, Nucl. Phys. **A361**, 29 (1975).
[47] E. Chabanat, Ph.D. thesis, Lyon, 1995.
[48] G. Fricke *et al.*, At. Data Nucl. Data Tables **60**, 177 (1995).
[49] B. Alex Brown, Phys. Rev. C **58**, 220 (1998).
[50] J. Friedrich and P.-G. Reinhard, Phys. Rev. C **33**, 335 (1986).
[51] A. Bouyssy, J.-F. Mathiot, and N. Van Giai, Phys. Rev. C **36**, 380 (1987).
[52] D. Vautherin and M. Veneroni, Phys. Lett. **26B**, 552 (1968).
[53] B. H. Brandow, Phys. Rev. **80**, 268 (1950).