HARTREE-FOCK MEAN-FIELD MODELS USING SEPARABLE INTERACTIONS

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An effective two-body nuclear interaction is presented which is a sum of terms separable in coordinate space. Calculations are made using this interaction of some doubly closed-shell spherical nuclei using many-body perturbation theory with the Hartree-Fock state as a reference state. It is demonstrated that the interaction gives good bulk properties in finite nuclei.

1 Force

Separable multipole forces have been used in the past as residual interactions to describe certain aspects of nuclei, such as deformation[1] or for shell-model calculations[2]. The infinite range of the separable multipole forces has led to their use in restricted space calculations. By introducing a density-dependence and extending the multipole force to include a monopole force, we perform full-space Hartree-Fock calculations to obtain bulk properties and use perturbation theory with the same interaction which generated the Hartree-Fock state to look at correlations. The two-body effective interaction is written

$$\begin{aligned}
V(r_1,r_2) &= W_a f_{\alpha_a}\rho^{\beta_a}(r_1)\rho^{\beta_a}(r_2)(1+a_a(\tau_1^+\tau_2^- + \tau_1^-\tau_2^+) + b_a\tau_{1z}\tau_{2z}) \\
&+ W_r f_{\alpha_r}\rho^{\beta_r}(r_1)\rho^{\beta_r}(r_2)(1+a_r(\tau_1^+\tau_2^- + \tau_1^-\tau_2^+) + b_r\tau_{1z}\tau_{2z}) \\
&+ k\nabla_1^2\rho(r_1)\nabla_2^2\rho(r_2) \\
&+ W_{D,p,n}A^{-\gamma}\sum_M(-1)^M\left(r_1\rho(r_1)Y_{1M}(\hat{r}_1)\right)\left(r_2\rho(r_2)Y_{1-M}(\hat{r}_2)\right) \\
&+ W_{Q,p,n}A^{-\gamma}\sum_M(-1)^M\left(r_1^2\rho(r_1)Y_{2M}(\hat{r}_1)\right)\left(r_2^2\rho(r_2)Y_{2-M}(\hat{r}_2)\right)
\end{aligned}$$

where the functions f_α are defined as

$$f_\alpha = \left[\int d^3 r\, \rho(r)^\alpha \right]^{-1}. \tag{1}$$

The first line in the potential is the attractive monopole term, and the second line is a functionally identical repulsive term. The third line is a surface term. The next line, being the term proportional to W_D, is the dipole term, and the term proportional to W_Q is the quadrupole interaction.

Furthermore, there is a one-body spin-orbit interaction

$$V_{\mathrm{s.o.}}(r) = c \frac{1}{r} \frac{\partial \rho}{\partial r} \vec{l} \cdot \vec{s}. \tag{2}$$

2 Calculations

Calculations have been made using this interaction in the Hartree-Fock (HF) approximation for closed-shell spherical nuclei. For such nuclei the direct contributions to the energy (and HF potential) from the multipole forces are zero. The exchange contribution is non-zero and, in principle, contributes to the spherical mean field, although for this report, the strengths for the multipole forces are set to zero. This is done since calculations of deformed nuclei and excited states, in which the multipole effects will be most obvious, have not yet been done, and only such calculations would allow one to fit the parameters for the multipole forces. The contribution of the monopole force to the HF energy and the HF potential is considered. Furthermore, correlations are calculated using the techniques of many-body perturbation theory[3] for the ground state energy. In contrast to realistic forces and most other effective interactions, such as the Skyrme interaction[4], this potential has a convergent perturbation series so diagrams may be evaluated order by order.

The parameters used are presented in Table 1. Table 2 compares experimental and calculated results of the rms charge radius in the HF approximation. It is expected that the corrections to such one-body observables are

W_a [MeV fm^3]	α_a	β_a	a_a	b_a	c [MeV fm^5]
-1568.0	2.0	1.0	0.4	-0.1125	180.0
W_r [MeV fm$^{3.84}$]	α_r	β_r	a_r	b_r	k [MeV fm^{10}]
1831.0	2.28	1.28	-0.4	0.08	8.0

Table 1. Monopole force parameters used in this paper.

Nucleus	r_{ch} calculated [fm]	r_{ch} experiment[5] [fm]
^{16}O	2.74	2.69
^{40}Ca	3.47	3.48
^{48}Ca	3.47	3.48
^{90}Zr	4.28	4.27
^{114}Sn	4.64	4.60
^{208}Pb	5.50	5.50

Table 2. Charge radii for some spherical nuclei

much smaller than the corrections to many-body observables, such as the energy. Table 3 shows the binding energy for the same nuclei. The calculation includes the Coulomb interaction with the Coulomb exchange calculated using the Slater approximation. There is no centre-of-mass correction.

Table 4 shows some properties of infinite nuclear matter calculations performed with the same set of parameters as used for the finite nuclear calculations. The equilibrium density, ρ_0, is the density of nuclear matter at which the energy is minimized and a typical experimental value is 0.16 ± 0.02 fm^{-3}. k_F is the fermi momentum and is related directly to the density. ϵ_0 is the energy at this density, with a typical value from a fitted mass formula being -15.6 ± 0.2 MeV. The correct value of the nuclear incompressibility, K_∞, is less well known, but the result obtained with this separable force is very close to those inferred from observations of the breathing mode excitations and the best fits with other effective interactions. The parameter a_s is the asymmetry energy. It is the coefficient of the asymmetry term in the semi-empirical mass formula, and its experimental value is around 30 MeV.

Nucleus	E_{HF}	E_2	E_3	Experiment[6]
^{16}O	-101.7	-2.95	1.08	-127.7
^{40}Ca	-340.3	-2.27	0.14	-342.0
^{48}Ca	-408.5	-6.00	0.68	-416.2
^{90}Zr	-786.1	-4.04	0.28	-783.9
^{114}Sn	-975.4	-4.19	0.29	-971.6
^{208}Pb	-1633.3	-5.18	0.15	-1636.4

Table 3. Binding energy contributions from Hartree-Fock and perturbation theory. All energies are in MeV

ρ_0 [fm^{-3}]	k_F [fm^{-1}]	ϵ_0 [MeV]	K_∞ [MeV]	a_s [MeV]
0.151	1.310	-15.69	220.10	29.22

Table 4. Nuclear matter properties

3 Discussion

The results calculated in Hartree-Fock order give quite a good description of the spherical nuclei presented. By using a density-dependent effective interaction, the total energy and the radius can simultaneously be fitted, and the separable form results in small correlations in perturbation theory. The energies up to third order agree with experiment within about 1% except for the lightest nucleus, ^{16}O, which is quite under-bound. This may be due to the omission of the centre-of-mass correction or a deficiency in the force. If the latter, the inclusion of multipole correlations may provide a solution or, alternatively, the inclusion of pairing. The quality of the fit to radii is slightly better than that to energy. In particular, the lack of increase in charge radius between ^{40}Ca and ^{48}Ca is reproduced. ^{16}O is somewhat too diffuse, which is not surprising given its under-binding.

The nuclear matter properties are all very reasonable. There is no contribution to nuclear matter binding energy per particle from perturbation theory, which one could have suspected from the fact that the lowest-order correction to the total energy of finite nuclei stays about the same as the number of particles increases and the higher-order corrections become smaller.

4 Conclusion

An effective interaction has been developed which can be used to calculate the properties of nuclei across the periodic table. The force has the advantage that the perturbation series seems to converge quickly so that the interaction may be used to calculate both the mean field properties and correlations beyond the mean-field using standard many-body perturbation theory. With the calculation of deformed nuclei, the parameters of the multipole forces may be fixed and perturbation calculations developed for excited state properties.

Acknowledgments

This work was supported in part through grants DE-FG02-96ER40963 and DE-FG02-94ER40834 from the U.S. Department of Energy. Oak Ridge National Laboratory (ORNL) is managed by Lockheed Martin Energy Research Corp. for the U.S. Department of Energy under contract number DE-AC05-96OR22464.

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