N=Z and proton-rich nuclei in the Hartree-Fock mean field model with a separable nucleon-nucleon interaction

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Abstract. A new model for the effective two-body nucleon-nucleon interaction has been recently successful in calculation of ground state properties of spherical, doubly closed shell nuclei from ^{16}O to ^{208}Pb [1] and nuclear matter and neutron star properties [2]. The application of the density dependent finite range separable monopole (SMO) interaction has been now extended to axially symmetrical deformed nuclei [3]. In the present paper we report on HF+BCS calculation of ground-state properties of even-even spherical and deformed $N = Z$ and proton-rich nuclei between the $N = Z$ and the proton-drip line for $28 \leq Z \leq 50$. The SMO results shown include total energy surfaces and deduced shapes, single-particle energies, two-dimensional distribution of nucleon densities, charge radii and two-proton separation energies. A comparison is made with results obtained using the SkO Skyrme interaction and some other theoretical models as well as with experimental data, where available.

HARTREE-FOCK CALCULATION USING THE MONOPOLE SEPARABLE NUCLEON-NUCLEON INTERACTION FOR AXIALLY DEFORMED NUCLEI

The separable monopole interaction

This interaction consists of two main parts, attractive (a) and repulsive (r) which have the same mathematical form for the density and isospin dependence and differ only in the values of adjustable parameters. Having attractive and repulsive terms with different ranges is a common feature of density-dependent effective interactions and it is these terms which are responsible for most of the binding energy in finite nuclei and for the volume energy in nuclear matter. To describe better surface properties of nuclei, a third term is added, depending on the second derivative of density.

Each term in the expression for the interaction is separable in the space coordinates of individual nucleons (and in isospin where applicable). This is the essential new property of this effective nucleon-nucleon interaction which makes it suitable for building a perturbation series in powers of the strength of the SMO interaction in order to include correlations in finite nuclei, beyond the mean field, with convergent results.

In coordinate space, the SMO is written as [1]

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

where the function f_ξ is defined as

$$f_\xi = \left[\int d^3\vec{r}\,\rho^{\alpha_\xi}(\vec{r})\right]^{-1}, \qquad (2)$$

for subscripts $\xi = a, r$. $\rho(\vec{r}_i)$ are nuclear densities, t are isospin operators and W_ξ, α_ξ, β_ξ, a_ξ, b_ξ and k are adjustable parameters.

In addition, we adopt the standard form of the spin-orbit interaction as used in mean-field calculations with the Skyrme interaction [17]:

$V_{ls} = c(\nabla\rho\cdot\sigma)(\sigma\cdot\nabla)$(3)

which provides an energy

$E_{ls} = -c\int d^3\vec{r}\,\rho\nabla\mathcal{J}$
(4)

and a contribution to the mean field of

$U_{ls} = c\nabla\mathcal{J}$,
(5)

where $\nabla\mathcal{J}$ is the spin-orbit current. The constant c in the above equations stands for the strength of the spin-orbit potential and corresponds to $t_4/2$ in the notation of Skyrme interactions. The Coulomb interaction which also has to be included in the model, is treated in the standard way and both direct and the exchange terms (in the Slater approximation) contribute to the total energy. The set of parameters SMO2 [2] was used in the present work. Both direct and exchange terms of the interaction are included into the Hartree-Fock equations.

Pairing had to be added to the model for correct treatment of open-shell nuclei. We follow the method of Bender et al. [15] who use the HF+BCS approximation and parametrise the effective δ-force pairing interaction in terms of a local pairing energy functional

$$\mathcal{E} = \frac{1}{4}\sum_{q\in p,n}\int d^3\vec{r}\chi_q^*(\vec{r})\chi_q(\vec{r})G_q(\vec{r}), \tag{6}$$

where $\chi_q(\vec{r})$, the local part of the pair density matrix, is expressed in terms of single-particle Hartree-Fock wave functions and pairing amplitudes u and v. The pairing strength G_q is dependent on nucleon density as

$$G_q(\vec{r}) = V_{0,q}\left[1-\left(\frac{\rho(\vec{r})}{\rho_0}\right)\right] \tag{7}$$

where $V_{0,q}$ are constants fitted to empirical pairing gaps of selected nuclei and ρ_0=0.16 fm^{-3} is the nuclear saturation density. This method treats pairing as a valence-particle effect and supresses to a large extent contributions from unbound continuum states close to the Fermi surface. This effect is in principle smaller for finite range forces [19]. Instead of a rather cumbersome implementation of these forces, the finite range effect can be simulated by introducing smooth energy-dependent cut-off weights (form-factors) F_a in evaluation of the local pair density $\chi_q(\vec{r})$ [15, 16]. The parameters of F_a are the width of the energy range of pairing active states and the average level density in the vicinity of the Fermi surface. These are adjusted to include approximately one additional shell above the Fermi energy.

The computer code developed for calculation of properties of axially deformed nuclei in Hartree-Fock + BCS model with a Skyrme effective interaction, used recently for calculation of shape-coexistence effects in light and medium neutron rich nuclei [17], has been adapted for the separable monopole interaction (Eq. 1). In this code the calculation is performed on a grid in cylindrical coordinates r, z, ϕ, with imposed symmetry with respect to the z-axis.

Calculated properties

After adding a quadrupole constraint $\hat{Q} \propto r^2 Y_{20}$ to the HF field, a systematic survey has been performed of ground state properties of N=Z even-even nuclei in the region 28≤Z≤50 and neutron-deficient nuclei between the N=Z line and the two-proton drip line towards the limits of nuclear existence. The calculated deformed shapes are characterized by a dimensionless quadrupole mass deformation parameter

$$\beta_2 = \sqrt{\frac{\pi}{5}}\frac{<r^2Y_{20}>}{A<r^2>} \tag{8}$$

where $<r^2>$ is the mean square radius of the mass distribution. Deformation parameters β_2^π (β_2^ν) of the proton (neutron) distributions were defined in an analoguous way. We do not consider β_4 deformation parameters in the present work (although their values have been calculated) as they are much less clearly connected to experimental data. Mean square radii are calculated in the usual way for the total, proton and neutron distributions

[17]. The correction for the finite size of the proton is included in the radius of the charge distribution as

$$r_{\rm ch}^2 = r_{\rm p}^2 + \underbrace{r_{\rm ch,p}^2}_{0.743\,{\rm fm}^2} - \frac{N}{Z}\underbrace{r_{\rm ch,n}^2}_{0.119\,{\rm fm}^2} \quad , \tag{9}$$

where $r_{\rm ch,p/n}$ are the nucleon radii.

The SkO Skyrme interaction [17] has been selected to demonstrate the similarities and differences between results obtained with the separable SMO model and a Skyrme model. This modern parametrisation has been used rather recently to study shape coexistence within the self-consistent Hartree-Fock method in N = 20, 28, 40 and 56 regions and belongs to the class of Skyrme interaction which behave well in calculation of nuclear matter and neutron star properties [18]. The total energy as a function of quadrupole deformation β_2 for ^{56}Ni, ^{60}Zn, ^{64}Ge, ^{68}Se, ^{72}Kr, ^{76}Sr, ^{80}Zr, ^{84}Mo, ^{88}Ru, ^{92}Pd, ^{96}Pd and ^{100}Sn in the SMO and SkO Skyrme models are shown in Fig. 1. The SMO model predicts a gradual departure from sphericity with increasing softness and prolate-oblate shape coexistence which starts at Z=32, peaks at large prolate deformation of ^{76}Sr and ^{80}Zr and decreases to zero at Z=44. The SkO Skyrme model predicts softer shape of ^{56}Ni, prolate-oblate shape coexistence in ^{60}Zn and ^{64}Ge with tendency to oblate shapes which develops in ^{68}Se and ^{72}Kr. For ^{76}Sr and heavier even-even N=Z nuclei up to ^{100}Sn the Skyrme model predicts well defined spherical shapes. As expected, our calculation shows that the proton and neutron matter separately follows the same pattern of shapes as the mass distribution. The calculated values of deformation parameter β_2, corresponding to the minimum total energy, are summarized in Table. 1 in comparison with results of some other model calculations. We notice that if there is a discrepancy in extracted values of β_2 between the SMO model and some of the other calculations, usually the SMO indicates two coexisting minima and one of them will be in agreement with the rest. This may indicate that there is delicate balance between calculated coexisting minima in all models. It would be useful if the deformation corresponding to the two lowest energy minima in all models was always given.

The present model is not adapted for a proper calculation of odd-A nuclei as yet and cannot be used to calculate one-proton separation energy, but allows predictions of the two-proton drip line. The results are shown in Fig. 2 and are in a good agreement with predictions of the other current models.

It is interesting to study the predicted development of nuclear shapes beyond the 2p drip-line. The nature of the proton-drip line is different from the neutron drip-line because in proton rich nuclei the proton decay occurs via tunneling of protons through the Coulomb potential barrier rather then leaving the nucleus freely when it becames unbound. Mean field calculations of this kind are technically demanding as a special care must be given to ensure that calculation of such exotic systems is meaningful. Standard nuclear models are designed for more ordinary systems with parameters fitted to properties of doubly closed shell nuclei. We present total energy surfaces for $^{58-76}$Sr nuclei with the SMO (left) and SkO Skyrme model (right) in Fig. 3. There is a difference between the predictions of the two models. SMO model predicts development of well defined deformed shapes with decreasing neutron number. On the contrary, the SkO Skyrme model indicates spherical shapes of proton-rich Sr isotopes well beyond the proton drip-line. An important observable closely connected to nuclear shapes is the

TABLE 1. Quadrupole deformation parameters of N=Z nuclei as calculated in different nuclear models.

A	Element	SMO	SkO [17]	MSk7 [6]	RMF [5]	FRDM [7]
60	Zn	0.0	-0.16 0.20 (0.439)	0.12	0.17	0.18
64	Ge	0.12 -0.16 (0.130)	-0.24 0.20 (0.008)	-0.19	0.22	0.22
68	Se	0.40 -0.20 (0.518)	-0.24 0.20 (0.032)	-0.25	-0.28	0.29
72	Kr	0.44 -0.24 (1.744)	-0.20 0.12 (0.778)	-0.20	-0.36	-0.34
76	Sr	0.48 -0.28 (2.398)	-0.12 0.48 (1.435)	0.42	0.41	0.42
80	Zr	0.44 -0.28 (2.104)	0.0	0.40	0.44	0.43
84	Mo	0.36 -0.24 (0.709)	0.0	0.0	-0.25	0.053

mean-square radius of nucleon density distributions in atomic nuclei. We compare in Fig. 4 the increase of the charge radius with increasing neutron defficiency taking the radius of ^{76}Sr as a base line. The two models, the SMO and SkO Skyrme model, predict very similar trends for both charge and neutron radii. No experimental data on radii exist in this region to date.

Whilst bulk deformation parameters and r.m.s.radii show limited sensitivity to details of nuclear models, the nucleon density distribution itself, in particular its spatial angular distribution is more interesting. In Fig.5 we show the calculated projection of the proton density distribution onto the rz plane (in cylindrical coordinates r, z, ϕ) for oblate and prolate minima of the total energy surface of ^{76}Sr. Taking z as the symmetry axis, individual single-particle orbitals will be spread from the origin depending upon the value of the orbital angular momentum $\mathbf{l}$. The resulting total distribution depends on the occupied single particle states close to the Fermi surface. This is illustrated in the lower part of Fig.5. Both for the oblate and prolate minimum of the total energy surface, the dominant contribution to the maximum density comes mainly from particles occupying high l orbitals $f_{5/2}$ and $g_{9/2}$. The occupation of the orbitals is of course smeared out due to the pairing interaction.

The distinctive sensitivity of the calculated density distribution to the single-particle spectrum makes it a powerful tool in distinguishing between models for the effective nucleon-nucleon interaction. Ground state proton and neutron density distributions differ considerably between the SMO model and the Skyrme SkO [17] model, as illustrated in Figs. 6,7. Data are shown for the stable spherical nucleus ^{88}Sr (N=50), the N=Z ^{76}Sr

(N=38) nucleus, and the drip-line nucleus ^{68}Sr (N=20). Interesting spatial distributions for protons and neutrons can be seen for ^{68}Sr, indicating overlapping orbitals, in the SMO model. The Skyrme model predicts development of spherical shapes at the drip-line and beyond, in variance with the SMO model which indicates increasing quadrupole deformation with decreasing neutron number.

CONCLUSIONS

We have shown that the newly developed SMO interaction describes N=Z and proton rich nuclei in a Hartree-Fock+BCS model giving predictions which are very similar to those of other mean-field models based on very different physics. This is true for observables obtained from one-body densities like nuclear shapes and mean radii of the charge and neutron distributions. These observables are therefore not useful criteria for selection between different models. On the contrary, the angular distribution of the proton density, which is in principle measurable directly, is very sensitive to details of the single particle spectra calculated using different nucleon-nucleon interactions. It may be that real progress in eliminating inadequate theories will require a new generation of difficult but possible experiments. Angular distribution of charge density in nuclei oriented in space, probed by a well tuned electron beam, is one of the challenges.

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REFERENCES

1. Stevenson, P., Strayer, M. R. and Rikovska Stone, J.,*Phys. Rev.*, **C63**, 054309 (2001)
2. Rikovska Stone, J., Stevenson, P. D. and Strayer, M. R.,*Phys. Rev.*, **C65**, 064312 (2002)
3. Stevenson, P. D., Rikovska Stone, J. and Strayer, M. R.,*Phys. Lett.*, **B545**,291 (2002)
4. Lalazissis, G. A. and Sharma, M. M., *Nucl. Phys.*, **A586**, 201 (1995)
5. Lalazissis, G. A., Raman, S. and Ring, P., *ADNDT*, **71**, 1 (1999)
6. Goriely, S., Tondeur, F. and Pearson, J. M., *ADNDT*, **77**, 311 (2001)
7. Moller, P., Nix, J. R., Meyers, W. D. and Swiatecki, W. J., *ADNDT*, **59**, 185 (1995)
8. Petrovici, A., Schmid, K. W. and Faessler, A.,*Nucl Phys.*, **A605**, 290 (1996)
9. Sarriguren, P., Moyay de Guerra, E. and Escuderos, A., *Nucl. Phys.*, **A658**, 13 (1999)
10. Engel, J., Langanke, K.-H. and Vogel, P., *Phys. Lett.*, **B389**, 211 (1996)
11. Yamagami, M., Matsuyanagi, K. and Matsuo, M., *Nucl. Phys.*, **A693**, 579 (2001)
12. Lister, C. J. et al., *Phys. Rev.*, **C42**, R1191 (1990)
13. Bucurescu, D., et al., *Phys. Rev.*, **C56**, 2497 (1997)
14. Marginean, N., et al., *Phys. Rev.*, **C63**, 031303(R) (2001)
15. Bender, M., Rutz, K.,Reinhard, P.-G. and Maruhn, J. A., *Eur. Phys. J.*, **A8**,59 (2000)
16. Krieger, S. J., Bonche, P., Flocard, H., Quentin, P. and Weiss, M. S., *Nucl. Phys.*, **A517**, 275 (1990)

17. Reinhard, P.-G., Dean, D. J., Nazarewicz, W., Dobaczewski, J., Maruhn, J. A. and Strayer, M. R., *Phys. Rev.*, **C60**, 014316 (1999)
18. Rikovska Stone, J., Miller, J. C., Koncewicz, R., Stevenson, P. D. and Strayer, M. R., submitted to *Phys. Rev. C*
19. Dobaczewski, J., Nazarewicz, W., Werner, T. R., Berger, J. F., Chinn, C. R. and Decharge, J., *Phys. Rev.*, **C53**, 2809 (1996)
20. Beiner, M., Flocard, H., Van Giai, N. and Quentin, P., *Nucl. Phys.*, **A236**, 269 (1974)
21. Van Giai, N. and Sagawa, H., *Phys. Lett.*, **106B**, **379** (1981)