

## SHELL-MODEL CALCULATIONS WITH A SKYRME-TYPE EFFECTIVE INTERACTION

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Shell-model calculations for the  $s$ - $d$  shell nuclei and Sn isotopes are performed using Hartree-Fock wave functions and two-body matrix elements based upon the SGII Skyrme-type density-dependent interaction. We reproduce the spectra of several nuclei from the beginning to the end of the  $s$ - $d$  shell. The experimental pairing gaps for the Sn isotopes are also obtained from calculations in the generalized seniority scheme using the same interaction. We find that the lower power of the density dependence associated with the SGII interaction is essential for obtaining realistic energy spectra in this wide range of mass.

It has been a long-standing problem to establish an effective interaction which can be used both for the calculation of the saturation properties and the excitation spectra of finite nuclei. A fundamental approach is based on reaction matrix theory [1,2]. Namely, an effective interaction is determined from the phase shifts of nucleon-nucleon scattering, and then a  $G$ -matrix calculation is carried out to obtain the two-body matrix elements for the structure calculations. However, this bare  $G$ -matrix does not give a proper account of the phenomenological two-body matrix elements. It has been pointed out [2] that the effect of core polarization must be included in order to obtain a reasonable success in the structure calculations. However, one must take into account the convergence properties of the perturbation expansion, and this leads to difficult and time-consuming computations for open-shell nuclei.

Vautherin and Brink [3] have proposed a simple interaction, the Skyrme interaction, which has been very successful for Hartree-Fock (H-F) calculations of many nuclei. With a proper parametrization, this interaction gives satisfactory results both for the saturation properties of nuclear matter and the properties of the giant resonances. The advantage provided by Skyrme interactions over other interactions, that have an explicit finite range, is that the computations for

the Hartree-Fock potentials and two-body matrix elements can be carried out relatively fast. However, it is clear that this interaction is not useful for shell-model calculations since previous parameter sets of the Skyrme interactions with a three-body term show a strong anti-pairing effect [4].

In this paper we will show that the extended Skyrme interaction proposed in ref. [5] provides reasonable particle-particle as well as hole-hole spectra without the need for the addition of any explicit core-polarization corrections. The modification consists of allowing for a lower power of the density dependence and for a small density-dependent spin-exchange mixture. Other types of extended Skyrme interactions have been proposed. Waroquier et al. [6] have suggested adding a momentum-dependent three-body or density-dependent term. The particle-particle matrix elements obtained with this interaction are similar to those obtained from a bare  $G$ -matrix, and realistic particle-particle spectra could be obtained only after adding core-polarization corrections [6]. This seems inconsistent in the sense that the Skyrme parameters have been fitted to the properties of nuclei such as  $^{16}\text{O}$ ,  $^{40}\text{Ca}$  and  $^{208}\text{Pb}$  with the assumption that these nuclei have closed-shell configurations and hence, the interaction should already implicitly contain the effects

of core polarization. We note that the extended Skyrme interactions of refs. [5,6] both give satisfactory results for the particle-hole interaction properties (e.g. the incompressibility coefficient and the Landau-Migdal parameters) without the need for explicit core-polarization corrections.

We will present calculations based on the parameter set SGII from ref. [5]. The calculations are performed in the following way. First, the spherical H-F equation is solved to obtain the single-particle energies (s.p.e.) and radial wave functions. Next, the two-body matrix elements for the Skyrme-type interactions are calculated by using these H-F wave functions. Thus, all ingredients of our shell-model calculations are derived from the SGII interaction. We will present results for several sd shell nuclei and for several Sn-isotope nuclei. For the sd shell-model calculations discussed below we have chosen to use experimental single-particle energies so that we can concentrate on the properties of the residual interaction in the comparisons. In the case of SGII, the difference between the H-F and experimental s.p.e. are  $-2.9$ ,  $-1.6$  and  $-0.7$  MeV for the  $1d_{5/2}$ ,  $1d_{3/2}$  and  $2s_{1/2}$  states in  $^{16}\text{O}$ , respectively, and  $0.0$ ,  $0.0$  and  $1.4$  MeV for these holes in  $^{40}\text{Ca}$ .

The Skyrme interaction SGII is written explicitly as

$$\begin{aligned} V(\mathbf{r}_1, \mathbf{r}_2) = & t_0(1 + x_0 P_\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) \\ & + \frac{1}{6} t_3(1 + x_3 P_\sigma) \rho^\alpha \delta(\mathbf{r}_1 - \mathbf{r}_2) \\ & + \frac{1}{2} t_1(1 + x_1 P_\sigma) (\mathbf{k}'^2 + \mathbf{k}^2) \delta(\mathbf{r}_1 - \mathbf{r}_2) \\ & + t_2(1 + x_2 P_\sigma) \mathbf{k}' \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k} \\ & + iW_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{k}' x \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k}, \end{aligned} \quad (1)$$

where  $\mathbf{k} = (\vec{\nabla}_1 - \vec{\nabla}_2)/2i$  and  $\mathbf{k}' = -(\vec{\nabla}_1 - \vec{\nabla}_2)/2i$ . The parameters of the SGII force are  $t_0 = -2645$  MeV fm<sup>3</sup>,  $x_0 = 0.09$ ,  $t_1 = 340$  MeV fm<sup>5</sup>,  $x_1 = -0.0588$ ,  $t_2 = -41.9$  MeV fm<sup>5</sup>,  $x_2 = 1.425$ ,  $t_3 = 15\,595$  MeV fm<sup>(1+ $\alpha$ )3</sup> and  $x_3 = 0.06044$ , respectively. The density dependence and the spin-orbit coupling are taken to be  $\alpha = 1/6$  and  $W_0 = 105$  MeV fm<sup>5</sup>. We can compare these to the parameters of the density-dependent SIII interaction [7] which is often used in the literature:  $t_0 = -1128.75$  MeV fm<sup>3</sup>,  $x_0 = 0.45$ ,  $t_1 = 395.0$

MeV fm<sup>5</sup>,  $x_1 = 0.0$ ,  $t_2 = -95.0$  MeV fm<sup>5</sup>,  $x_2 = 0/0$ ,  $t_3 = 14\,000$  MeV fm<sup>6</sup>,  $x_3 = 1.0$ ,  $\alpha = 1$  and  $W_0 = 120$  MeV fm<sup>5</sup>, respectively. The first two terms in eq. (1) are the most important for the saturation properties, and the momentum-dependent terms are introduced to take into account the effect of the finite-range force and are important for the surface properties. The latter give rise to an effective mass of  $m^*/m = 0.79$  for SGII and  $0.76$  for SIII in nuclear matter. The strength of the spin-orbit coupling is determined from the energy splitting of  $1p_{1/2}$  and  $1p_{3/2}$  states in  $^{16}\text{O}$ .

Let us now discuss the results for two particles and two holes in the sd shell. In fig. 1, we show the spectra for  $^{18}\text{O}$  and  $^{38}\text{Ar}$  obtained with the SIII and SGII interactions in comparison with the results obtained with Wildenthal's interaction [8] and experiment. Wildenthal's interaction (W) was obtained empirically by fitting the two-body matrix elements to sd shell binding energies and excitation energies. The two-body matrix elements were calculated using the radial wave functions as obtained from the H-F calculations for the ground states of  $^{16}\text{O}$  and  $^{36}\text{Ar}$ . In  $^{18}\text{O}$ , the calculated spectra with the SIII interaction is very much compressed and the energy of the first  $0^+$  state is even higher than that of the first  $2^+$  state. On the other hand, the SGII interaction gives results very similar to those based on Wildenthal's matrix elements. As noted above, we used the density-dependent type SIII force, instead of the three-body type. Both versions are equivalent for the H-F calculations of close-shell nuclei [3,4,6], but the three-body force gives much poorer results for two-body matrix elements than the present ones obtained from the density-dependent SIII force [4]. We see also that the spectrum of the two-hole states in  $^{38}\text{Ar}$  obtained by the SIII force is more compressed than the other two calculations. We find that all versions of the Skyrme interactions in refs. [3,7] give similar poor results for the spectra of these two-particle and two-hole systems.

In order to study more details of our interaction, some two-body matrix elements for the sd shell configurations are given in table 1 together with those of Wildenthal [8] and Daehnick [10]. We can see a large cancellation between the first

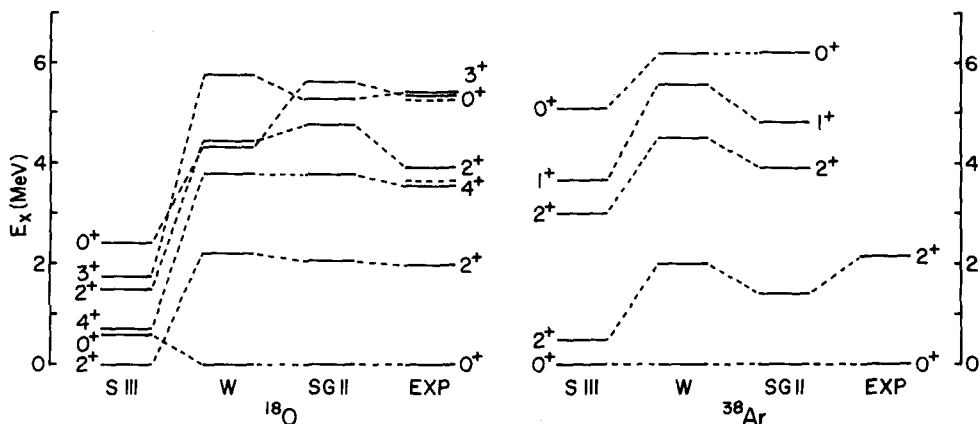


Fig. 1. The calculated energy spectra of  $^{18}\text{O}$  and  $^{38}\text{Ar}$  obtained with the Skyrme interactions SIII and SGII and with phenomenological matrix elements of Wildenthal (W) are compared with experiment [9]. For  $^{38}\text{Ar}$  only the levels below 3 MeV excitation are given. The states denoted by dashed lines are known to be predominantly core-excited  $4p-2h$  configurations which are outside the configuration space of present calculations.

two terms of eq. (1) for every matrix element reflecting the attractive and repulsive characters of two forces which are necessary to obtain the proper saturation. The momentum-dependent term is always repulsive and behaves like an anti-pairing force. The two-body spin-orbit interaction has an isovector character and is also repulsive for the pairing matrix element. Summing up all four contributions in table 1, our two-body matrix

elements are reasonably close to the phenomenological values given in the last two columns. This is the main reason why our calculation shows good agreement with the experimental spectra. However, we notice two shortcomings of our matrix elements: (1) the relative strengths of the matrix elements for  $(1d_{5/2})^2$ - and  $(1d_{3/2})^2$ -multiplets are very close to the phenomenological values, but the absolute magnitudes tend to be larger; (2) our

Table 1  
Two-body matrix elements for some sd-shell configurations. The phenomenological values are taken from ref. [8] (W) and ref. [10] (D)<sup>a)</sup>.

	$J$	$T$	$\delta$	$\rho^\alpha \delta$	$k^2 + k' \cdot k$	$L \cdot S$	SGII	W	D
$(1d_{5/2})^2$ [ $^{16}\text{O}$ core]	1	0	-15.55	9.33	2.26	0.	-3.96	-1.63	-3.62
	3	0	-8.73	5.24	1.04	0.	-2.46	-1.50	-1.65
	5	0	-13.65	8.19	0.83	0.	-4.63	-4.22	-3.87
	0	1	-23.92	15.23	4.35	0.63	-3.72	-2.82	-3.00
	2	1	-5.47	3.49	0.52	-0.34	-1.80	-1.00	-1.12
	4	1	-2.23	1.45	0.01	-0.09	-0.90	-0.16	0.26
$(1d_{3/2})^2$ [ $^{40}\text{Ca}$ core]	1	0	-8.13	5.36	0.82	0.	-1.96	-1.13	-1.31
	3	0	-8.13	5.36	0.38	0.	-2.40	-2.30	-2.45
	0	1	-11.32	7.91	1.44	0.53	-1.45	-1.75	-2.51
	2	1	-2.26	1.58	0.18	0.04	-0.47	-0.05	0.15

<sup>a)</sup>The matrix elements of Daehnick were deduced from the analysis of one-nucleon transfer data. His results are similar to those obtained in the analysis of Schiffer and True [11]. Since these experiments are sensitive to  $l$  transfer rather than  $j$  transfer, in cases where there is strong configuration mixing involving both  $j = l \pm 1/2$  orbits it may be difficult to extract reliable  $j-j$  coupled matrix elements. This may be the main reason for the differences between the matrix elements of Daehnick and those of Wildenthal, in particular for the case of  $(1d_{5/2})^2$   $J = 1$ .

matrix elements for the ( $J = 1, T = 0$ ) and ( $J = 3, T = 0$ ) channels of the  $(1d_{5/2})^2$  configuration differ significantly from those of Wildenthal.

In figs. 1 and 2 the calculations are compared with experiment. The experimental excitation energies of the isoscalar ( $T = 0$ ) and the isovector ( $T = 1$ ) states in  $^{36}\text{Ar}$  are both reproduced well by the SGII force. The matrix elements of the two-body interaction for the other sd shell nuclei were obtained from a linear interpolation of the SGII H-F results for  $^{16}\text{O}$  and  $^{40}\text{Ca}$ . (It is interesting to note that the  $^{16}\text{O}/^{40}\text{Ca}$  ratio of 0.76 for the monopole energy of the SGII matrix elements summed over all three sd shell orbits, is the same result obtained from Wildenthal's empirical mass dependence of  $A^{0.3}$  for the two-body matrix elements [8].) The calculated (experimental) excitation energies of the first  $2^+$  states in other nuclei are 2.47 (1.63) MeV for  $^{20}\text{Ne}$ , 1.96 (1.37) MeV for  $^{24}\text{Mg}$ , and 2.22 (2.23) MeV for  $^{32}\text{S}$ . In spite of the disagreement noted above for some of the  $T = 0$  matrix elements, the spectra obtained for the even-even sd shell nuclei look quite reasonable. The calculated level spacings for nuclei in the lower sd shell are spread out as compared to experiment. This discrepancy might be related to the strong collective nature of the nuclei in this mass region.

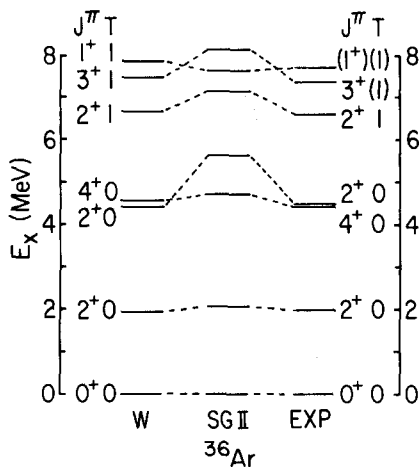


Fig. 2. Calculated and experimental energy spectra of  $^{36}\text{Ar}$ . The data are taken from ref. [9].

Relative to  $^{16}\text{O}$  and  $^{40}\text{Ca}$ , the calculated binding energies for the open-shell nuclei are systematically too large relative to experiment, up to about 0.5 MeV/A for nuclei in the center of the sd shell. This is related to an overestimate of the absolute magnitude of the two-body matrix elements. However, the H-F wave functions reproduce the empirical RMS charge radii to within about 2% for these open shell nuclei [12]. This aspect of our calculation is important for the study of transition densities of excited states.

Arima et al. [13] have claimed that for a density-dependent finite-range interaction it is impossible to reproduce a realistic spectra for both beginning and end shell nuclei. The SIII interaction, for example, reproduces a correct ordering of the  $0_1^+$  and  $2_1^+$  levels in the end shell nucleus  $^{38}\text{Ar}$  while in  $^{18}\text{O}$  the ordering of the levels is completely off. However, our interaction gives good agreement for the spectra in both regions of the sd shell. The lower power for the density dependence in the SGII interaction might be crucial for obtaining reasonable spectra both at the beginning and the end of the shell.

In order to further investigate the SGII interaction, we have also performed the calculations for the Sn isotopes. Some results are shown in fig. 3 and compared with experimental data. We use the generalized-seniority scheme [14] for these calculations, taking five single-particle states ( $3s_{1/2}$ ,  $2d_{3/2}$ ,  $1g_{7/2}$ ,  $1h_{11/2}$  and  $2d_{5/2}$ ) for the neutron

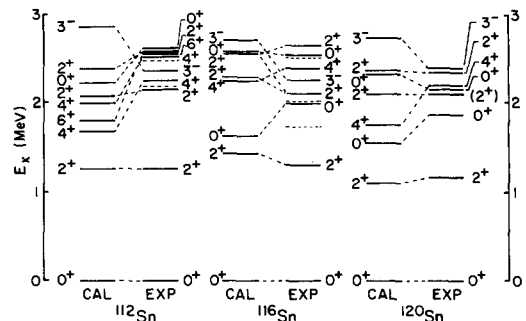


Fig. 3. Energy spectra for the Sn isotopes. The data are taken from refs. [15-17] for  $^{112}\text{Sn}$ , refs. [9,15] for  $^{116}\text{Sn}$  and ref. [9] for  $^{120}\text{Sn}$ . The states denoted by dashed lines are identified as two-proton core-excited states [17,18] which are outside the configuration space of present calculations.

Table 2

Two-body matrix elements in the Sn region. The coupling constant of the surface  $\delta$ -force [19] is taken to be  $A_T = 0.18$  MeV [14].

	$J$	$T$	SGII	surface- $\delta$
$(1g_{7/2})^2$	0	1	-0.73	-0.72
	2	1	-0.39	-0.17
	4	1	-0.21	-0.08
	6	1	-0.13	-0.04
$(2d_{5/2})^2$	0	1	-0.66	-0.54
	2	1	-0.44	-0.12
	4	1	-0.23	-0.05

configurations. Taking the H-F single-particle energies, the calculated (experimental) quasi-particle excitations in  $^{115}\text{Sn}$  are 0.0 (0.0) MeV for  $3s_{1/2}$ , 0.45 (0.61) MeV for  $1g_{7/2}$ , 0.52 (0.50) MeV for  $2d_{3/2}$ , 1.10 (0.71) MeV for  $1h_{11/2}$  and 1.30 (0.99) MeV for  $2d_{5/2}$ . For the structure calculations discussed below, we have lowered the  $h_{11/2}$  s.p.e. by 400 keV. The energy gaps between the  $0^+$  and  $2^+$  states are well reproduced by the calculations for all mass numbers. The best agreement occurs in  $^{120}\text{Sn}$  where the second and third  $0^+$  and  $2^+$  states are also very close to experiment. Although the  $3^-$  states are always higher than experiment, this may be reasonable since the higher  $1\hbar\omega$  and  $3\hbar\omega$  configurations are important for this collective state. We show some matrix elements for  $^{116}\text{Sn}$  in table 2 together with those of the surface  $\delta$ -interaction [19].

In summary, we have studied the shell-model calculations for the sd shell nuclei and Sn isotopes using the two-body matrix elements of the Skyrme force SGII. Our calculations are in good agreement with experimental data in both mass regions without changing any parameter of the interaction. The lower power ( $\alpha = 1/6$ ) of the density-dependent force is important to obtain realistic energy spectra both in the beginning and the end of the sd shell without the need for any explicit core-

polarization correction. We obtain reasonable matrix elements not only for the sd shell configurations but also for the Sn isotopes with the same set of parameters. It would be interesting to apply our interaction to nuclei in other mass regions and study whether further improvements in the Skyrme parameters can be obtained by fitting to binding energies and excitation energies of levels in open-shell nuclei.

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