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1974 J. Phys. A: Math. Nucl. Gen. 7 372

(http://iopscience.iop.org/0301-0015/7/3/008)

J. Phys. A: Math., Nucl. Gen., Vol. 7, No. 3, 1974. Printed in Great Britain.

Scheme of the approximate relativistic theory of the nucleus I. Calculation of the single-particle basis hamiltonian from internucleon interactions

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Received 23 July 1973

Abstract. The approximate relativistic equation (relativistically invariant to within terms in v^2/c^2) for a system of nucleons is used in this paper as the starting point to obtain the nuclear average field, isobaric-spin potential and spin–orbit potential. Calculations are carried out in the framework of the Hartree–Fock approximation. Accounting for the wavefunction of proper symmetry noticeably improves the agreement with experiment. The nuclei ^{41}Ca and ^{209}Pb are considered for illustration, different variants of the two-particle interactions of the OBEP type being utilized.

1. Introduction

Both the nuclear structure theory and the theory of internucleon interactions are developing at present, to a large extent independently and loosely coordinated. Chiefly employed in the theory of nuclear structure are either simplified model interactions or interactions in the form of the conventional mixture of the forces of Wigner, Bartlett, Heisenberg and Majorana with a large number of fitting parameters. At the same time the theory of internucleon interactions has made essential progress in recent years, being based increasingly on the meson theory of nuclear forces in the variant of the so-called one-boson exchange potentials—the OBEP—which include pseudoscalar (P), scalar (S) and vector (V) mesons (Bryan and Scott 1964, 1969, Green and Sawada 1967, Ingber 1968). However, only the nucleon–nucleon scattering data (and partly, the deuteron data) are utilized for constructing and fitting the OBEP, nuclear structure being, as a rule, ignored.

It is evident that such a gap is harmful both for the theory of internucleon interactions and for the theory of nuclear structure and that a sufficiently trustworthy picture may be obtained only by correlation and coordination of the two theories.

In the paper by Krutov (1973) the program of construction of the approximate relativistic theory of the nucleus (to be referred to as ART) was briefly formulated, it started from the *relativistic* (to within terms in v^2/c^2) two-nucleon equation of the Breit type (Breit 1937) taking into consideration all necessary intermediate mesons and resonances. Use of the Hartree–Fock procedure for solving the many-nucleon problem was supposed to be the first step in the realization of the program with the further accounting for the

nondiagonal part of the interaction (ie, for the so-called 'residual interactions' in conventional terminology).

Execution of the program was started in Krutov and Savushkin (1973), where the single-particle spin–orbit potential V_{SO} and average field V_{av} were calculated starting from the nucleon–nucleon OBEP-type interactions, the values obtained for ^{41}Ca and ^{209}Pb being in reasonable agreement with the experimental values. However, calculations in that paper were performed in the framework of the Hartree approximation. In the present paper calculations of the spin–orbit potential V_{SO} and of the average field V_{av} are carried out in the Hartree–Fock approximation (§§ 2–4), which improves the agreement with experiment. Moreover, in the present paper we obtain the isobaric-spin potential V_{IS} (§§ 3, 4) by the Hartree–Fock method. Thus, in the present paper starting from the internucleon interactions we obtain the single-particle hamiltonian which forms the basis states for solving the many-nucleon problem.

In a subsequent paper (II) the authors intend (resting on the single-particle basis hamiltonian obtained in I) to consider the description of binding energies, spectra and states of nuclei in the framework of the ART. Special attention will be paid to formation of the so-called collective nuclear states.

Finally, in the third part of the paper (III) we shall revise the set of mesons and resonances of the OBEP variants utilized in I and II and refine the interaction in the sense of extension of the exchange potentials.

Actually, in the present paper I and in the subsequent paper II we utilize in the calculations the OBE potentials available from papers by Green and Sawada (1967) and Ueda and Green (1968). However, apart from the incomplete adequacy of the OBEP from a theoretical point of view, because of the nature of the OBEP approximation (ie assuming the hypothetical S meson etc) the OBE potentials should be fitted, as is evident from the paper by Krutov and Savushkin (1973) and from the present paper, not only to the nucleon–nucleon scattering data and deuteron data (as is done in papers by Green and Sawada 1967 and Ueda and Green 1968) but *simultaneously* to the calculations (with the OBEP) of the single-particle nuclear potential (spin–orbit potential, average field and isobaric-spin potential)†. It gives an additional criterion which is essential for the proper determination of internucleon interactions. It is just the inadequate choice of the mesons and resonances (besides the limitedness of the OBE potentials) which are available from the papers mentioned above and utilized here that causes the theoretical values V_{SO}, V_{av}, V_{IS} obtained in this paper to differ somewhat from experimental values (see the discussion in § 4). At the same time the difference may be considered as not being a matter of principle, and agreement between theory and experiment as rather satisfactory especially taking into account the fact that the theoretical values are obtained with the OBE potentials fitted to totally independent data on the nucleon–nucleon scattering. It shows once more that the concept of the OBE potentials is fruitful, but they also need refinement in the sense stated above.

At the same time the scheme of the ART in itself (the scheme of calculations of the single-particle basis hamiltonian, binding energies, nuclear spectra, transitions, etc from internucleon interactions) depends only slightly on the choice of mesons and resonances of the OBEP and will remain almost unaltered after subsequent refinement and revision of this choice. For this reason we considered it to be advisable to present the scheme of the ART and to perform calculations based on the available variants of the OBE potentials before accomplishment of the work on revision of the OBEP since this work is laborious and time consuming.

† And later to calculations of the binding energies, nuclear spectra and transitions as well.

2. Average field and isobaric-spin potential

The relativistic Breit-type equation (Breit 1937) with two-particle forces due to the exchange of pseudoscalar, vector and scalar mesons is the starting point for the present paper as well as for the previous one (Krutov and Savushkin 1973). This equation may be obtained by the method suggested by Fock (1934) and it is written for two nucleons, for example, in the paper by Green and Sawada (1967). For an A nucleon system it has the following form:

$$\left\{\sum_i^A (c\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + \beta_i mc^2) + \frac{1}{2}\sum_{i,k}^A \left[-\beta_i \cdot \beta_k \left(\sum_{\mathrm{S}} V_{ik}^{\mathrm{S}} + \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \sum_{\mathrm{S}\tau} V_{ik}^{\mathrm{S}\tau} \right) \right.\right.$$
$$+ (1 - \boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_k) \left(\sum_{\mathrm{V}} V_{ik}^{\mathrm{V}} + \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \sum_{\mathrm{V}\tau} V_{ik}^{\mathrm{V}\tau} \right)$$
$$\left.\left. + \beta_i \gamma_{5,i} \beta_k \gamma_{5,k} \left(\sum_{\mathrm{P}} V_{ik}^{\mathrm{P}} + \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \sum_{\mathrm{P}\tau} V_{ik}^{\mathrm{P}\tau} \right) \right] \right\} \phi = E\phi, \tag{1}$$

here $\gamma_5 = \beta\gamma^1\gamma^2\gamma^3$, $\boldsymbol{\gamma} = \beta\boldsymbol{\alpha}$, $\boldsymbol{\alpha}$ is the Dirac matrix vector; $\boldsymbol{\tau}_i$ is the isospin matrix of the ith nucleon; $\Sigma_{\mathrm{S}}, \Sigma_{\mathrm{V}}, \Sigma_{\mathrm{P}}$ indicate summation over isoscalar scalar, vector and pseudoscalar mesons, respectively; sums $\Sigma_{\mathrm{S}\tau}, \Sigma_{\mathrm{V}\tau}, \Sigma_{\mathrm{P}\tau}$ are related to isovector mesons with the same space–time transformation properties; ϕ is a relativistic wavefunction of an A-nucleon system, ie, the direct product of A bispinors; E is the total energy of a stationary state ϕ.

Two-particle potentials V_{ik} are the functions of the distance between the particles $r_{ik} = |\boldsymbol{r}_i - \boldsymbol{r}_k|$, they may have different representations but to obtain adequate fitting to the nucleon–nucleon scattering data (with the OBE potentials) the repulsive core should be brought into these functions in one form or another.

To try to solve the many-nucleon problem with equation (1) directly would be a fairly difficult, and at the same time unnecessary (because of the approximate nature of equation (1)), undertaking. That is why we reduce these equations to the v^2/c^2 limit, ie, we write them down for only the 'large' component (we designate it as ψ) of the wavefunction, excluding the 'small' component. After performing the reduction we obtain the approximate relativistic equation (relativistically invariant to within terms in v^2/c^2), which is the starting point for the subsequent investigation:

$$\left(\sum_i^A \frac{\boldsymbol{p}_i^2}{2m} + \frac{1}{2}\sum_{i,k}^A (V_{ik} + V_{ik}^{\mathrm{SO}} + \delta V_{ik}^{\mathrm{SO}} + \delta V_{ik}^{\mathrm{rel}}) \right) \psi = \epsilon\psi, \tag{2a}$$

$$V_{ik} = \sum_{\mathrm{S}} V_{ik}^{\mathrm{S}} - \sum_{\mathrm{V}} V_{ik}^{\mathrm{V}} + \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \left(\sum_{\mathrm{S}\tau} V_{ik}^{\mathrm{S}\tau} - \sum_{\mathrm{V}\tau} V_{ik}^{\mathrm{V}\tau} \right), \tag{2b}$$

$$V_{ik}^{\mathrm{SO}} = -\frac{\hbar}{8m^2c^2} \boldsymbol{r}_{ik} \times \boldsymbol{p}_{ik} \cdot (\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_k) \frac{1}{r_{ik}} \frac{\mathrm{d}}{\mathrm{d}r_{ik}} \left\{ \left(\sum_{\mathrm{S}} V_{ik}^{\mathrm{S}} + 3\sum_{\mathrm{V}} V_{ik}^{\mathrm{V}} \right) \right.$$
$$\left. + \boldsymbol{\tau}_i \cdot {}_k \left[\sum_{\mathrm{S}\tau} V_{ik}^{\mathrm{S}\tau} + \sum_{\mathrm{V}\tau} \left(3 + 4\frac{f^{\mathrm{V}\tau}}{g^{\mathrm{V}\tau}} \right) V_{ik}^{\mathrm{V}\tau} \right] \right\}, \tag{2c}$$

$$\delta V_{ik}^{\mathrm{SO}} = -\frac{\hbar}{8m^2c^2} \boldsymbol{r}_{ik} \times (\boldsymbol{p}_i + \boldsymbol{p}_k) \cdot (\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_k) \frac{1}{r_{ik}} \frac{\mathrm{d}}{\mathrm{d}r_{ik}} \left[\left(\sum_{\mathrm{S}} V_{ik}^{\mathrm{S}} - \sum_{\mathrm{V}} V_{ik}^{\mathrm{V}} \right) + \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k \left(\sum_{\mathrm{S}\tau} V_{ik}^{\mathrm{S}\tau} - \sum_{\mathrm{V}\tau} V_{ik}^{\mathrm{V}\tau} \right) \right] \tag{2d}$$

In equation (2) $\boldsymbol{p}_{ik} = \boldsymbol{p}_i - \boldsymbol{p}_k$ ($\boldsymbol{r}_{ik}$ is defined similarly); $\delta V_{ik}^{\mathrm{rel}}$ are the relativistic corrections to the internucleon interaction of the order v^2/c^2 which do not possess the form of the spin–orbit forces (we shall discuss these corrections in II); $f^{\mathrm{V}\tau}$ and $g^{\mathrm{V}\tau}$ are, respectively, the tensor and vector coupling constants of vector isovector mesons with nucleons. In equation (2) we have divided the spin–orbit interaction into two parts: the galilean invariant operator V_{ik}^{SO} and the operator $\delta V_{ik}^{\mathrm{SO}}$ which is non-galilean invariant. The non-galilean invariant forces may appear only in a system consisting of more than two particles, ie, in the case when each pair is moving in the field formed by the remainder of the nucleus.

Equation (2*a*) has the form of the conventional Schrödinger equation for an A-nucleon system. In the framework of the Hartree–Fock approximation all nucleons are considered as moving in a total, generally speaking, nonlocal potential, and the wavefunction ψ is represented by a Slater determinant of single-particle wavefunctions which depend on the space, spin and isospin coordinates of one nucleon. These single-particle wavefunctions are the solutions of the following Hartree–Fock equations:

$$\left(\frac{\boldsymbol{p}^2}{2m}\psi_i(\xi) + \sum_{k\leqslant A}\int \mathrm{d}\xi'\psi_k^*(\xi')\hat{V}(\xi,\xi')(\psi_k(\xi')\psi_i(\xi) - \psi_i(\xi')\psi_k(\xi))\right) = \epsilon_i\psi_i(\xi), \quad (3)$$

where ϵ_i are the single-particle nucleon energies, ξ designates the set of the space, spin and isospin coordinates of a nucleon, $\int \mathrm{d}\xi$ includes integration over space and summation over spin and isospin variables.

Let us consider the contribution of the static terms to the average field, ie, in equation (3) we take $\hat{V}(\xi,\xi') = V_{ik}$. In the present paper we take into account the proper symmetry of the wavefunction and in this sense we speak about the Hartree–Fock approximation although here, as in Krutov and Savushkin (1973), we do not carry out the self-consistency procedure. We suppose that the nucleon density distribution has the following form:

$$\rho(\boldsymbol{r}) = \sum_{\substack{k\leqslant A\\ \sigma,\tau}} |\psi_k(\boldsymbol{r},\sigma,\tau)|^2, \quad (4)$$

where summation over spin and isospin variables is performed, ψ_k are solutions of equation (3).

To calculate the average field, we shall utilize the short-range limit for the two-particle forces given by (2*b*), ie, we shall assume that the single-particle wavefunctions ψ_i do not change essentially at distances of effective radius of nuclear forces (2*b*). Since only heavy mesons and resonances are important in our calculations (the exchange by the π meson makes no contribution to the basis single-particle hamiltonian in the static limit), the short-range approximation is sufficiently justified to be used for our purposes. In the framework of this approximation the nonlocal Hartree–Fock potential is reduced to the local one and we obtain the following equation for an even–even nucleus or for an odd nucleon in an odd nucleus:

$$\left(\frac{\boldsymbol{p}^2}{2m} + V_{\mathrm{av}}(\boldsymbol{r}) + V_{\mathrm{IS}}(\boldsymbol{r})\right)\psi_i(\xi) = \epsilon_i\psi_i(\xi), \quad (5a)$$

where

$$V_{\mathrm{av}}(\boldsymbol{r}) = 3\pi\rho(\boldsymbol{r})\int_0^\infty \left[\left(\sum_{\mathrm{S}} V_{ik}^{\mathrm{S}}(x) - \sum_{\mathrm{V}} V_{ik}^{\mathrm{V}}(x)\right) - \left(\sum_{\mathrm{S}\tau} V_{ik}^{\mathrm{S}\tau}(x) - \sum_{\mathrm{V}\tau} V_{ik}^{\mathrm{V}\tau}(x)\right)\right] x^2\,\mathrm{d}x, \quad (5b)$$

$$V_{IS}(r) = \tau_3^i \pi(\rho_n(r) - \rho_p(r)) \int_0^\infty \left[\left(\sum_S V_{ik}^S(x) - \sum_V V_{ik}^V(x) \right) \right.$$
$$\left. - 5 \left(\sum_{S\tau} V_{ik}^{S\tau}(x) - \sum_{V\tau} V_{ik}^{V\tau}(x) \right) \right] x^2 \, dx, \tag{5c}$$

where $\rho_n(r)$ and $\rho_p(r)$ are the neutron and proton densities, respectively. It should be noticed that in contrast to Krutov and Savushkin (1973) we have here separated the isobaric-spin potential V_{IS} from V_{av}. Obtaining equations (5) we made use of the following relation:

$$\sum_{\substack{k \leqslant A \\ \sigma\tau}} \psi_k^*(r, \sigma, \tau) \sigma \psi_k(r, \sigma, \tau') = 0 \tag{6}$$

where τ' may be both different from and equal to τ. Relation (6) follows from the fact that in an even–even nucleus the state obtained from an occupied state by the time-reversal operator is also occupied (if we consider the average field for an odd nucleon in the Hartree–Fock approximation, we may, as formerly, perform summation over the even–even core).

As is seen from equations (5), the difference between the Hartree–Fock and Hartree approximations (cf equation (26*b*), Krutov and Savushkin 1973) is essential in calculation of V_{av}; as for the isobaric-spin potential V_{IS}, the Hartree–Fock and Hartree methods lead in general to quite different results (cf equation (5*c*) of the present paper and equation (26*b*) of Krutov and Savushkin 1973).

Values of V_{av} and V_{IS} calculated with different variants of OBEP are presented in § 4.

3. Relativity and spin–orbit interaction in nuclei

Consider now calculation of the spin–orbit potential on the basis of equations (2) using the technique outlined in the preceding paper (Krutov and Savushkin 1973) in which the spin–orbit interaction in the nucleus has been considered in the Hartree approximation. In the present paper we make use of the Hartree–Fock approximation.

First of all we notice that the operator δV_{ik}^{SO} plays a less important role than the galilean-invariant operator V_{ik}^{SO} since δV_{ik}^{SO} is proportional to the *difference* of the contributions from scalar and vector mesons. As was shown by Krutov and Savushkin (1973), the value of the spin–orbit potential is determined by the sum of the contributions from scalar and vector mesons whereas the average field is determined by the difference of their contributions. Thus, the contribution from δV_{ik}^{SO} to the spin–orbit splittings is approximately of the same magnitude as that from the Thomas coupling, ie, is by one order of magnitude smaller than the contribution from V_{ik}^{SO}. Therefore we shall omit this operator in this section (the contribution from this operator to the spin–orbit splittings is taken into account, however, in the results given in table 1, see also appendix 1).

The spin–orbit splittings are expressed in terms of the spin–orbit force contributions to the single-particle energies in the following manner:

$$\Delta E_{nl}^{SO} = \epsilon_i^{SO}(j = l - \tfrac{1}{2}) - \epsilon_i^{SO}(j = l + \tfrac{1}{2}) \tag{7a}$$

where in the Hartree–Fock approximation

$$\epsilon_i^{SO} = \sum_{k \leqslant A} (\langle ik | V_{ik}^{SO} | ik \rangle - \langle ik | V_{ik}^{SO} | ki \rangle). \tag{7b}$$

Table 1. Spin–orbit splittings obtained in the framework of the Hartree–Fock approximation for the following variants of two-body forces: a, Green and Sawada (1967); b, Ueda and Green (1968) (model II); c, Ueda and Green (1968) (model III); d, Stagat *et al* 1971). The spin–orbit splittings in the Hartree approximation are given in parentheses†

	a	b	c	d	Experimental data
$\Delta E^{SO}_{1f}(^{41}Ca)$	13·8 (9·32)	3·55 (1·75)	4·63 (2·42)	3·06 (1·57)	6·50
$\Delta E^{SO}_{2p}(^{41}Ca)$	3·30 (2·22)	0·843 (0·415)	1·10 (0·577)	0·728 (0·373)	2·00
$\Delta E^{SO}_{2g}(^{209}Pb)$	3·53 (2·22)	0·845 (0·422)	1·11 (0·588)	0·736 (0·380)	2·47
$\Delta E^{SO}_{1i}(^{209}Pb)$	11·2 (7·08)	2·70 (1·35)	3·56 (1·87)	2·34 (1·20)	4·57
$\Delta E^{SO}_{3d}(^{209}Pb)$	2·03 (1·28)	0·487 (0·243)	0·644 (0·339)	0·423 (0·218)	0·98

† All quantities are given in MeV. The relative thickness of the surface layer τ is assumed to be 0·4.

The direct matrix element in (7*b*) is the same as that calculated formerly in the Hartree approximation (Krutov and Savushkin 1973). So it remains to calculate the exchange matrix element. To this end we write the wavefunction for two nucleons in the form

$$|ik\rangle = [\varphi^{(+)}_{ik}(\boldsymbol{r}, \boldsymbol{r}') + \varphi^{(-)}_{ik}(\boldsymbol{r}, \boldsymbol{r}')][\chi^{S=1}_{ik}(\sigma, \sigma') + \chi^{S=0}_{ik}(\sigma, \sigma')]\chi_i(\tau)\chi_k(\tau') \tag{8a}$$

with

$$\varphi^{(\pm)}_{ik}(\boldsymbol{r}, \boldsymbol{r}') = \pm\varphi^{(\pm)}_{ik}(\boldsymbol{r}', \boldsymbol{r}), \tag{8b}$$

$$\chi^{S}_{ik}(\sigma, \sigma') = (-1)^{S+1}\chi_{ik}(\sigma', \sigma), \tag{8c}$$

ie, χ^S_{ik} is the spin wavefunction with spin S; $\varphi^{(+)}_{ik}$ contains, obviously, only even relative angular momentum states of nucleons, and $\varphi^{(-)}_{ik}$ contains only odd ones.

The interaction V^{SO}_{ik} acts only in $S = 1$ states because of the presence of the operator of doubled spin $(\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_k)$. Moreover, we may take into account the interaction only in relative P states according to the short-range approximation adopted. Introducing the notation

$$V^{SO}_{ik} = V^{SO}_0 + \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k V^{SO}_\tau$$

one gets

$$\langle ik|V^{SO}_0|ki\rangle = -\langle ik|V^{SO}_0|ik\rangle\delta_{\tau_i,\tau_k}, \tag{9a}$$

$$\langle ik|\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k V^{SO}_\tau|ki\rangle = -\langle ik|\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_k V^{SO}_\tau|ik\rangle(1 - 3\delta_{\tau_i,-\tau_k}). \tag{9b}$$

Taking into account all said above, the contributions from corresponding mesons to single-particle energies in the Hartree–Fock approximation may be expressed in terms of those in the Hartree approximation in the following manner:

$$(\epsilon^{SO}_i(S))_{HF} = (\epsilon^{SO}_i(S) + \epsilon^{SO}_{i\tau}(S))_H, \tag{10a}$$

$$(\epsilon_i^{SO}(V))_{HF} = (\epsilon_i^{SO}(V) + \epsilon_{i\tau}^{SO}(V))_H, \tag{10b}$$

$$(\epsilon_i^{SO}(S\tau))_{HF} = (3\epsilon_{i\tau}^{SO}(S\tau) - \epsilon_i^{SO}(S\tau))_H, \tag{10c}$$

$$(\epsilon_i^{SO}(V\tau))_{HF} = (3\epsilon_{i\tau}^{SO}(V\tau) - \epsilon_i^{SO}(V\tau))_H, \tag{10d}$$

where $\epsilon_{i\tau}^{SO}$ denotes the contribution only from nucleons of the same kind (neutrons or protons) as the nucleon in state i.

When the wavefunctions of proper symmetry are used we define the single-particle spin–orbit potential as follows

$$V_{SO}(i) = \sum_{k \leqslant A} \int d\xi' \psi_k^*(\xi') V_{ik}^{SO}(\xi, \xi') \psi_k(\xi') - \frac{1}{\psi_i(\xi)} \sum_{k \leqslant A} \int d\xi' \psi_k^*(\xi') V_{ik}^{SO}(\xi, \xi') \psi_i(\xi') \psi_k(\xi). \tag{11}$$

We confine ourselves to nuclei with one nucleon (in state i) above the doubly closed shell containing $A-1 = N+Z$ particles and use, as well as above, the short-range approximation. Then after having used the same technique as that in Krutov and Savushkin (1973), one obtains†

$$V_{SO}(i) = \frac{\pi}{4} \frac{\hbar^2}{m^2c^2} \frac{1}{r} \frac{d\rho}{dr} \int_0^\infty \frac{d}{dx} \left\{ \left(\sum_S V_{ik}^S(x) + 3 \sum_V V_{ik}^V(x) \right) + \left[\sum_{S\tau} V_{ik}^{S\tau}(x) + \sum_{V\tau} \left(3 + 4 \frac{f^{V\tau}}{g^{V\tau}} \right) V_{ik}^{V\tau}(x) \right] \right\} x^3 \, dx \left(1 - \tau_3^i \frac{N-Z}{3A} \right) \boldsymbol{l} \cdot \boldsymbol{\sigma} \tag{12}$$

where it is assumed that

$$\rho_n(r) = \frac{N}{A} \rho(r), \qquad \rho_p(r) = \frac{Z}{A} \rho(r). \tag{13}$$

From (12) the relation for the spin–orbit splittings of the same neutron and proton states, evidently, follows

$$\frac{\Delta E_{nl}^{SO}(\text{neutron})}{\Delta E_{nl}^{SO}(\text{proton})} = \frac{A+N}{A+Z} > 1. \tag{14}$$

Notice that relation (14) does not correspond to the empirical analysis of Ross *et al* (1956) which was utilized by Krutov (1973). However, the isobaric-spin dependence of the spin–orbit splittings has not yet been determined reliably.

4. Calculation of spin–orbit splittings, average field, and isobaric-spin potential with OBEP interaction: discussion

In §§ 2–3 we have obtained the basis single-particle hamiltonian in the form:

$$H(i) = \frac{\boldsymbol{p}^2}{2m} + V_{av}(i) + V_{IS}(i) + V_{SO}(i) \tag{15}$$

where $V_{av}(i)$, $V_{IS}(i)$, and $V_{SO}(i)$ are given by equations (5*b*), (5*c*), and (12), respectively. Consider now numerical calculations of the spin–orbit splittings ΔE_{nl}^{SO} and the values

† See also the derivation of equation (10) where the technique of calculating the exchange term is given.

of the average field and isobaric-spin potential using different two-body forces. We employ in these calculations the same computational model as in the paper by Krutov and Savushkin (1973), ie, we assumed a trapezoidal density distribution for $\rho(r)$ and make use of infinite-rectangular-well single-particle wavefunctions in calculating ΔE_{nl}^{SO}.

The results of calculations of the spin–orbit splittings in the Hartree–Fock approximation obtained with different OBE potentials are given in table 1. Our present calculations are carried out for the relative thickness of the surface layer $\tau = 0{\cdot}4$ so that $R = 1{\cdot}33A^{1/3}$ fm corresponds approximately to $R_{1/2} = 1{\cdot}07A^{1/3}$ fm (see Krutov and Savushkin 1973).

The results of calculations of V_{av} and V_{IS} are given in table 2. Let us dwell on the isobaric-spin potential. Assuming (13) one finds

$$\frac{V_{IS}(r)}{V_{av}(r)} = \tau_3^i \frac{N-Z}{4A} \frac{\frac{4}{3}\int_0^\infty [(\Sigma_S V_{ik}^S(x) - \Sigma_V V_{ik}^V(x)) - 5(\Sigma_{S\tau} V_{ik}^{S\tau}(x) - \Sigma_{V\tau} V_{ik}^{V\tau}(x))]x^2\,dx}{\int_0^\infty [(\Sigma_S V_{ik}^S(x) - \Sigma_V V_{ik}^V(x)) - (\Sigma_{S\tau} V_{ik}^{S\tau}(x) - \Sigma_{V\tau} V_{ik}^{V\tau}(x))]x^2\,dx}$$

$$= \tau_3^i \frac{N-Z}{4A} \frac{v_{IS}^{eff}}{V_{av}^{eff}}, \tag{16}$$

where v_{IS}^{eff}† is just the symmetry–energy parameter denoted usually as V_1. To determine the value of this parameter, a very simple 'occupation-number method' has been suggested (Krutov and Savushkin 1969) (note that here and in the paper by Krutov and Savushkin 1969, the signs of τ_3 and $2t_3$ are chosen differently). According to this method, V_1 is obtained from the difference of the proton and neutron well depths, this difference

Table 2. The values of the neutron average field and isobaric-spin potential obtained in the framework of the Hartree–Fock approximation for the same variants of two-body forces as in table 1. To make comparison with the results obtained in the Hartree approximation (Krutov and Savushkin 1973) (figures in parentheses), more convenient we included V_{IS} into V_{av} in this table†

	a	b	c	d	Experimental data
$\tilde{V}_{av}(^{41}Ca)$	−34·0 (−45·3)	−56·2 (−73·3)	−60·8 (−85·4)	−20·8 (−29·8)	
$\tilde{V}_{av}(^{209}Pb)$	−31·7 (−45·3)	−52·6 (−72·7)	−57·7 (−86·1)	−19·9 (−30·4)	
$V_{av}^{eff}(^{41}Ca)$	−27·1 (−36·1)	−44·8 (−58·4)	−48·4 (−68·0)	−16·6 (−23·7)	−46·1
$V_{av}^{eff}(^{209}Pb)$	−25·3 (−36·1)	−41·9 (−57·9)	−45·9 (−68·6)	−15·8 (−24·2)	−53·4
$v_{IS}^{eff}(^{209}Pb)$	36·1 (0)	64·4 (8·11)	46·7 (−12·7)	13·8 (−8·98)	79·4

† All quantities are given in MeV. The relative thickness of the surface layer τ is assumed to be 0·4. The experimental values of V_{av}^{eff} are taken from the proton scattering data (Greenlees and Pyle 1966), for neutrons the experimental values of $|V_{av}^{eff}|$ for ^{208}Pb must be somewhat smaller than 53·4.

† The value v_{IS}^{eff} is determined similarly to V_{av}^{eff} by the relation $\tilde{v}_{IS}(R_{1/2})^2 = v_{IS}^{eff}(R_{1/2}^{eff})^2$ since, in accordance with (13), the effect of the isobaric-spin potential reduces to lowering or raising the nuclear potential well without its distortion.

being determined by the difference of the neutron and proton numbers N and Z:

$$v_{IS}^{eff} = V_1 = (\Delta V_{pn} + V_{coul}) \frac{2A}{A-2Z}. \tag{17}$$

In accordance with (17) one has $v_{IS}^{eff} = 79{\cdot}4$ MeV for ^{209}Pb. This value is just given in table 2 as the experimental one. The data given in tables 1 and 2 show that the Hartree–Fock approximation gives essentially better results than the Hartree approximation. Indeed, the Hartree–Fock approximation leads to larger values of ΔE_{nl}^{SO}, affecting the value of V_{av} to a lesser extent (if compared to the Hartree results). The Hartree approximation is not effective in calculating the isobaric-spin potential, whereas the Hartree–Fock approximation is able to give a result close to the experimental one (for two-body forces b and c, see table 2).

Accounting for the proper symmetry of the wavefunctions for determining the basis single-particle hamiltonian (carried out in the present paper) considerably reduces the number of possible sources of discrepancy between theoretical and experimental values. The remaining origins are the following: (i) the short-range approximation; (ii) approximate character of the computational model; (iii) limiting to the first step of the iteration self-consistent procedure; (iv) neglect of the 'residual interactions'; (v) insufficiency of the OBE potentials.

The short-range approximation has been discussed above and the corresponding corrections will be considered in the future. The approximate character of the computational model has been discussed by Krutov and Savushkin (1973) and shown to cause errors which are not very essential. Consideration of the density in the form of equation (4) and modelling this density by the trapezoidal distribution with the half density radius $R_{1/2} = 1{\cdot}07A^{1/3}$ fm enables us to avoid the principal difficulties of the iteration procedure and leads to sufficiently accurate results even in the first stage. The neglect of the residual interactions for near-magic nuclei ^{41}Ca and ^{209}Pb is hardly essential for the quantities calculated in the present paper. This follows, for example, from the fact that pairing-correlation effects do not occur in these nuclei (occupation numbers are equal to 1 or 0).

Therefore the main source of the discrepancy between the quantities ΔE_{nl}^{SO}, V_{av}^{eff} and V_{IS}^{eff} calculated in this paper and the experimental ones is, probably, insufficiency of the OBE potentials used. This conclusion is supported also by the fact that different OBE potentials yield very different results (see tables 1 and 2). As was mentioned in the introduction, calculation of V_{SO}, V_{av}, V_{IS} should be one of the criteria for choosing the proper OBEP. In particular, our calculations show (see case d in tables 1 and 2) that the 'realistic' OBE potential of Stagat *et al* (1971) is inferior when applied to the many-particle problem (or more accurately, in calculating the single-particle basis hamiltonian). However, to avoid misunderstanding, it should be noted that our results are, in general, the arguments in favour of the OBE potentials, since the discrepancy of the calculated and experimental quantities is not very significant. This discrepancy is not a matter of principle, the ways to eliminate it being clear. Meanwhile, our calculations performed for usual Wigner, Bartlett, Heisenberg and Majorana mixture forces indicate (see Krutov and Savushkin 1973) that these forces cannot, in principle, give reasonable values simultaneously for the average field and spin–orbit splittings, if we start from the approximately relativistic equation of the Breit type. The use of such forces in nuclear-structure theory is, from our point of view, a palliative. In simplified working models, more simple interactions appear to be advisable for usage (see, eg Krutov 1973). In more precise theories the OBEP interactions and still more exact forces are to be employed.

Appendix 1. Non-galilean part of the spin–orbit interaction

In this appendix we discuss the non-galilean spin–orbit interaction δV_{ik}^{SO} in equations (2). The contribution from this interaction to spin–orbit splittings may be evaluated in the Hartree approximation in the same manner as that from the galilean interaction. Therefore it is sufficient to consider only the exchange matrix elements

$$\langle ik|\delta V_{ik}^{SO}|ki\rangle.$$

The consideration is simplified greatly in the case of using the L–S coupling. Of course, the j–j coupling is more preferable for nuclei; however, the more approximate accounting for the interaction δV_{ik}^{SO} may be justified by the small value of this operator. Furthermore, the L–S coupling appears to be correct, as will be shown below, for the so-called spin-saturated nuclei (ie, the nuclei with completely occupied or completely empty spin–orbit doublets). Since addition of an extra nucleon does not affect the spin–orbit splittings in the Hartree–Fock approximation (and supposing that the wavefunctions of the other nucleons are not altered by the extra nucleon), we may apply the consideration given below also to spin-saturated-plus-one-nucleon nuclei (ie, for ^{41}Ca).

Consider the sum of the exchange matrix elements over the spin-saturated core, ie, over all nucleons except one in state i:

$$\bar{\delta}_i = \sum_{k \leq A-1} \langle ik|\delta V_{ik}^{SO}|ki\rangle. \tag{A.1}$$

For spherical-symmetry reasons we have

$$\Delta = \sum_i \bar{\delta}_{i(j=l+\frac{1}{2})} + \sum_i \bar{\delta}_{i(j=l-\frac{1}{2})} = 2(l+1)\bar{\delta}_{j=l+\frac{1}{2}} + \bar{\delta}_{j=l-\frac{1}{2}} 2l. \tag{A.2}$$

Since according to (A.1) and (A.2) the quantity Δ contains summation over spin saturated sets of states (both k and i), for states k and i we may employ the L–S scheme instead of the j–j scheme. Suppose, in addition, the radial wavefunctions for $j = l \pm \frac{1}{2}$ are close to each other. Then the matrix element $\langle ik|\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_k|ki\rangle$ is equal to zero. Indeed, the third components of $\boldsymbol{\sigma}_i$ and $\boldsymbol{\sigma}_k$ cancel, the other two components do not contribute because of the spin-projection conservation. Therefore we have $\Delta = 0$.

On the other hand, for state i with the projection of the magnetic quantum number $m = j = l + \frac{1}{2}$ both schemes (L–S and j–j) coincide. Therefore, due to spherical symmetry we have $\bar{\delta}_{j=l+\frac{1}{2}} = 0$. From the latter relation, equation (A.2) and $\Delta = 0$, one obtains $\bar{\delta}_{j=l-\frac{1}{2}} = 0$. Then we conclude that the exchange terms of δV_{ik}^{SO} do not contribute to the spin–orbit splittings for spin-saturated nuclei (as is also the case in utilizing the L–S coupling for spin-nonsaturated nuclei).

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