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Short-Range Correlations with Pseudopotentials. IV

AHMED OSMAN[1]

International Centre for Theoretical Physics, Trieste, Italy

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Abstract

Using a unitary model operator, the short-range correlations between nucleons in nuclei have been considered. To achieve healing in the wave functions, short-range pseudopotentials are required to be added to the nucleon–nucleon potential. With the introduction of the pseudopotentials, the matrix element for the effective interaction in nuclei is developed with correlated basis wave functions. The tensor forces and the short-range pseudopotentials are renormalized in second-order perturbation theory. Hartree–Fock calculations are carried out for the two finite closed-shell spherical nuclei ^{16}O and ^{40}Ca. The calculations of the resulting effective Hamiltonian are carried out with an effective interaction derived from the Tabakin potential. The present calculations of the binding energies per particle for the ^{16}O and ^{40}Ca nuclei are in agreement with the experimental measurements.

1. *Introduction*

From phase-shift analysis, it has been realized that the nucleon–nucleon interactions exhibit very strong repulsive nuclear forces at short distances. In that sense, the nuclear nucleon–nucleon potential is expressed as a long-range attractive potential surrounded by a very short-range repulsive potential. The presence of these short-range repulsive forces complicates the nuclear structure calculations in obtaining satisfactory values for the static properties of nuclei. The short-range correlations have been described by different interesting approaches that had been developed, such as the reaction matrix theories, the separation, the reference spectrum and the variational methods. In the case of nonlocal nucleon–nucleon interactions, it is found that the unitary model operator is more useful to take into account the short-range correlations in nuclei.

[1] Permanent address: Physics Department, Faculty of Science, Cairo University, Cairo, Egypt.

In three preceding papers (Osman, 1976a–c), referred to as I, II, and III, respectively, we considered the short-range correlations using a unitary model operator. Short-range pseudopotentials are required to be added to the short-range repulsive part of the nucleon–nucleon potential to achieve healing in the wave functions and to produce zero phase shift in the pair state. With these pseudopotentials, an effective Hamiltonian is obtained. The healing of the correlated wave functions, using the short-range pseudopotentials, is obtained taking into account the second-order terms from both the tensor forces and the pseudopotentials. Hartree–Fock calculations have been applied to obtain the binding energies per particle for the two finite closed-shell spherical nuclei ^{16}O and ^{40}Ca. The Hartree–Fock equations have been carried out using the Hamada–Johnston (1962), Yale group (Lasilla et al., 1962) and Reid (1968) potentials and also for a potential calculated by us (Osman, 1977) according to meson exchange between nucleons. Another effective potential for nucleon–nucleon calculations had been suggested by Tabakin (1964), which matches the different partial-wave nucleon–nucleon phase parameters. Tabakin defined a suitable set of separable potentials to produce a smooth two-body wave function. The Tabakin potential introduces a good interaction model because it lacks realistic short-range calculations which, however, are implicitly assumed to be of little importance for low-lying levels of nuclei. The model potential defined by Tabakin is taken to be separable of the Yamaguchi type (Yamaguchi, 1954; Yamaguchi and Yamaguchi, 1954[2]) as the sum of a short-range repulsive part plus a long-range attractive part.

In the present paper, the short-range correlations in nuclei are considered using a unitary model operator. Short-range pseudopotentials are added to the repulsive short-range part of the nuclear nucleon–nucleon potential to produce zero phase shift in the pair state. These pseudopotentials are required to be added to achieve healing of the correlated wave functions. The healing of the correlated wave functions, using the short-range pseudopotentials, is obtained taking into account the second-order terms from both the tensor forces and the pseudopotentials. The mathematical expressions for the procedure is given explicitly in our preceding papers I, II, and III. In the present work we calculate the binding energies per particle for the two finite closed-shell spherical nuclei ^{16}O and ^{40}Ca. In the present calculations, the Hartree–Fock equations are applied using the Tabakin potential for the nuclear nucleon–nucleon interaction. Corrections for both the Coulomb energy and the center-of-mass energy are also taken into account.

In Section 2 the Tabakin potential model used is introduced. Expressions for the effective Hamiltonian and the binding energy as an application of Hartree–Fock calculations are given in Section 3. Section 4 is left for calculations and discussion.

[2] These two articles will be referred to together simply as "Yamaguchi."

2. *The Tabakin Potential Model Used*

Tabakin suggested a potential model that is a nonlocal separable potential defined as

$$V(\mathbf{r}, \mathbf{r}') = \lambda \sum_{\alpha MLL'} [-g_{\alpha L}(r) g_{\alpha L'}(r') + h_{\alpha L}(r) h_{\alpha L'}(r')] \mathscr{Y}^{M}_{\alpha L}(\hat{\mathbf{r}}) \mathscr{Y}^{M}_{\alpha L'}(\hat{\mathbf{r}}') \tag{2.1}$$

where α denotes the quantum numbers JTS. The function $\mathscr{Y}^{M}_{\alpha L}(\hat{\mathbf{r}})$ is a normalized eigenstate of total angular momentum J and its Z component M; it is a combination of an orbital angular momentum state $Y^{M_L}_{L}(\hat{\mathbf{r}})$, and a total spin state $\chi^{M_S}_{S}$ and $\lambda = \hbar^2/m$ (m is the nucleon mass):

$$\begin{aligned} \mathscr{Y}^{M}_{\alpha L}(\hat{\mathbf{r}}) &= \mathscr{Y}^{M}_{JLS}(\hat{\mathbf{r}}) P_T \\ &= \sum_{M_S M_L} \langle M_L M_S \mid C_{LS} \mid JM \rangle \, Y^{M_L}_{L}(\hat{\mathbf{r}}) \, \chi^{M_S}_{S} P_T \end{aligned} \tag{2.2}$$

P_T is a projection operator that projects out an eigenstate of total isospin T, and its Z projection T_3 so that

$$P_{T'} \chi^{T_3}_{T} = \delta_{TT'} \chi^{T_3}_{T} \tag{2.3}$$

The complete partial-wave decomposition of the model potential expressed by equation (2.1), permits independent interactions in each allowed state. Forbidden states naturally have no interactions. The symbols $g_{\alpha L}(r)$ and $h_{\alpha L}(r)$ refer to the attractive and repulsive parts of the potential, respectively.

In the relative coordinates, the Schrödinger equation for such a nonlocal potential is

$$-\lambda \nabla^2 \psi_n(\mathbf{r}) + \int V(\mathbf{r}, \mathbf{r}') \psi_n(\mathbf{r}') \, d\mathbf{r}' = E_n \psi_n(\mathbf{r}) \tag{2.4}$$

where E_n is the total energy in the center-of-mass system $E_n = \lambda k_n^2$. Transforming to the momentum space representation, one has

$$\lambda (k_n^2 - k^2) \psi_n(\mathbf{k}) = \int d\mathbf{k}' V(\mathbf{k}, \mathbf{k}') \psi_n(\mathbf{k}') \tag{2.5}$$

with

$$\psi_n(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int e^{-i\mathbf{k}\cdot\mathbf{r}} \psi_n(\mathbf{r}) \, d\mathbf{r} \tag{2.6}$$

where $\hbar \mathbf{k}_n$ is the incident momentum.

Correspondingly, the potential in momentum space is

$$V(\mathbf{k}, \mathbf{k}') = \frac{2}{\pi} \lambda \sum_{\alpha MLL'} f^{\alpha}_{LL'}(k, k') \mathscr{Y}^{\alpha}_{ML}(\hat{\mathbf{k}}) \mathscr{Y}^{*\alpha}_{ML'}(\hat{\mathbf{k}}') \tag{2.7}$$

where

$$f^{\alpha}_{LL'}(k, k') = i^{L'-L} [-g_{\alpha L}(k) g_{\alpha L'}(k') + h_{\alpha L}(k) h_{\alpha L'}(k')] \tag{2.8}$$

In expression (2.8), the potentials $g_{\alpha L}(k)$ and $h_{\alpha L}(k)$ in their momentum representation are represented by the Yamaguchi form for the S and D states, where these potential functions have the expressions

$$\begin{aligned} g_0(k) &= \gamma(k^2 + a^2)^{-1} \\ h_0(k) &= \beta k^2 [(k-d)^2 + b^2]^{-1} [(k+d)^2 + b^2]^{-1} \\ g_2(k) &= \bar{\gamma} k^2 [(k-\bar{c})^2 + \bar{a}^2]^{-1} [(k+\bar{c})^2 + \bar{a}^2]^{-1} \\ h_2(k) &= \bar{\beta} k^2 [(k-\bar{d})^2 + \bar{b}^2]^{-1} [(k+\bar{d})^2 + b^2]^{-1} \end{aligned} \tag{2.9}$$

The parameters γ, β, a, and b correspond to potential strengths and ranges, and d is the hard-core radius.

3. *The Effective Hamiltonian and Binding Energy*

Using the same notations as in our papers I, II and III, an expression for the effective Hamiltonian is obtained considering only one- and two-particle interactions. This effective Hamiltonian H_{eff} is expressed as

$$\begin{aligned} H_{\text{eff}} = & \sum_{ij} a_i^\dagger \langle i|h_1|j\rangle a_j \\ & + \frac{1}{2!} \sum_{ijmn} a_i^\dagger a_j^\dagger \langle \Psi_{ij} | \nu_{12}^l - \nu_p + \nu_T^{\text{OD}} \\ & + \nu_T^{\text{OD}}(Q/e)\nu_T^{\text{OD}} + \nu_p(Q/e)\nu_p \,|\, \Psi_{mn}\rangle a_m a_n \end{aligned} \tag{3.1}$$

with the definition of each quantity here as presented in papers I, II, and III. In expression (3.1), ν_{12}^l stands for the long-range part of the nucleon–nucleon potential, ν_p is the short-range pseudopotential, and ν_T^{OD} is the off-diagonal part of the nucleon-nucleon potential which received contributions only from the tensor force.

$\nu_T^{\text{OD}}(Q/e)\nu_T^{\text{OD}}$ and $\nu_p(Q/e)\nu_p$ are the second-order terms in the off-diagonal tensor forces ν_T^{OD} and in the pseudopotentials ν_p, respectively. Following Kuo and Brown (1965), to consider the second-order terms, the Pauli principle projection operator Q and the appropriate energy denominator e are expressed as

$$Q(k, K, k_f) = \begin{cases} 0 & \text{for } k^2 + \frac{1}{4}K^2 < k_f^2 \\ 1 & \text{for } k - \frac{1}{2}K > k_f \\ (k^2 + \frac{1}{4}K^2 - k_f^2)/kK & \text{otherwise} \end{cases} \tag{3.2}$$

and

$$e = \frac{\hbar^2}{2m}(k_1^2 + k_2^2) + \Delta = \frac{\hbar^2}{m}(k^2 + \tfrac{1}{4}K^2) + \Delta \tag{3.3}$$

where the intermediate plane wave states of momenta $\mathbf{k}_1$ and $\mathbf{k}_2$ are introduced,

$$\mathbf{k} = \tfrac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$$
$$\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2 \tag{3.4}$$

and Δ is a measure of the binding of the interacting pair in the nucleus.

To apply the Hartree–Fock method to calculate the binding energy per particle, let us denote the single-particle potential by V, where

$$\langle i \mid V \mid j \rangle = \sum_{k=1}^{A} [\langle ik \mid v_{\text{eff}} \mid jk \rangle - \langle ik \mid v_{\text{eff}} \mid kj \rangle] \tag{3.5}$$

and if h is the kinetic energy operator, then the binding energy is given by

$$E_0 = \sum_{nn'} \rho_{n_1 n_1'} [\langle n_1 \mid h \mid n_1' \rangle + \tfrac{1}{2} \langle n_1 \mid V \mid n_1' \rangle] \tag{3.6}$$

where

$$\rho_{n_1 n_1'} = \sum_{k=1}^{A} C_{n_1}^{k} C_{n_1'}^{k} \tag{3.7}$$

and

$$\sum_{n_1'} [\langle n_1 \mid h \mid n_1' \rangle + \langle n_1 \mid V \mid n_1' \rangle] \; C_{n_1'}^{i} = \epsilon_i C_{n_1}^{i} \tag{3.8}$$

4. *Calculations and Discussion*

In the present work, calculations of the present proposed model are made to investigate short-range correlations in nuclei. Here, the nuclear nucleon–nucleon interaction is taken as the Tabakin (1964) potential model presented in Section 2 with two different sets of parameters due to Yamaguchi (1954), Yamaguchi and Yamaguchi (1954), and Breit et al. (1962). The two different representations of parameters are given in Table I. The pseudopotentials required to be added to achieve healing in the correlated wave functions have been calculated so as to produce zero phase shift in the pair state. These pseudopotentials have been calculated for different values of n and different values of the oscillator size parameter ν of the basis wave functions, which are taken as harmonic-oscillator wave functions. The calculated values of the required pseudopotentials are listed in Tables II–VI for the different S, P, and D states. The matrix elements of the first- and second-order terms have

TABLE I. Parameters of the nucleon–nucleon Tabakin potential

Potential parameters	a^{-1} fm	c^{-1} fm	b^{-1} fm	d^{-1} fm	V_γ MeV	V_μ MeV
Yamaguchi	0.752	0.125	–	–	113.9	660.5
Breit et al.	0.834	–	0.801	0.694	115.9	235.6

TABLE II. Pseudopotentials for the $^1S_0$ state. Healing distance = 1.02 fm, Tabakin potential (Yamaguchi)

	Pseudopotentials (MeV) for different ν (fm)			
n	1.48	1.76	2.16	2.38
0	−4.6	0.0	0.0	0.0
1	−25.1	−16.3	−10.3	−7.7
2	−53.5	−42.8	−22.1	−14.8
3	−85.9	−79.4	−41.9	−28.9
4	−131.2	−118.1	−65.4	−45.4

TABLE III. Pseudopotentials for the $^1S_0$ state. Healing distance = 1.02 fm, Tabakin potential (Breit et al.)

	Pseudopotentials (MeV) for different ν (fm)			
n	1.48	1.76	2.16	2.38
0	−5.6	0.0	0.0	0.0
1	−28.3	−20.5	−10.9	−7.9
2	−61.1	−50.4	−25.2	−16.1
3	−93.9	−83.6	−44.3	−30.3
4	−139.2	−127.7	−68.1	−46.6

TABLE IV. Pseudopotentials for the $^3S_1$ state. Healing distance = 1.05 fm, Tabakin potential (Yamaguchi)

	Pseudopotentials (MeV) for different ν (fm)			
n	1.48	1.76	2.16	2.38
0	−87.1	−79.2	−73.8	−69.9
1	−104.3	−94.1	−86.3	−81.1
2	−115.2	−108.8	−95.9	−90.3
3	−149.9	−123.5	−114.2	−108.5
4	−179.7	−139.4	−133.1	−126.8

TABLE V. Pseudopotentials for the $^3S_1$ state. Healing distance = 1.05 fm, Tabakin potential (Yamaguchi)

	Pseudopotentials (MeV) for different ν (fm)			
n	1.48	1.76	2.16	2.38
0	−105.4	−98.2	−89.8	−87.9
1	−126.1	−116.4	−106.5	−99.4
2	−148.3	−132.1	−115.1	−111.3
3	−183.8	−157.9	−142.2	−135.6
4	−225.5	−175.3	−166.7	−152.2

TABLE VI. Pseudopotentials for the P and D states. $n = 0$, $\nu = 1.76$ fm

States	Pseudopotentials (MeV)		
	Tabakin (Yamaguchi)	Tabakin (Breit et al.)	Healing distance (fm)
$^1P_1$	−586.3	−717.5	0.99
$^3P_0$	−214.8	−259.9	0.99
$^3P_1$	−223.1	−268.6	0.99
$^3P_2$	−12.4	−15.7	0.99
$^3D_1$	−45.1	−55.8	0.98
$^3D_2$	−185.8	−229.9	0.98
$^3D_3$	−182.4	−226.7	0.98
$^1D_2$	−11.5	−14.1	0.98

also been calculated. In our calculations, we considered the values for $\nu = 1.76$ fm, $\Delta = 20$ MeV, and $k_f = 1.4$ fm^{-1}. Kuo and Brown (1965) had shown that the values of k contributing to the integral are quite large, so the upper limit of the K integral could be taken as $2k_f$. Also, the value used for $\Delta = 20$ MeV is reasonable for the least tightly bound orbitals where one usually applies the shell theory. In our paper III, we found that increasing Δ by about 20 MeV yields a decrease in the second-order matrix element of about 5%. The change of k_f by 0.1 fm^{-1} introduces a change in the matrix elements of about 4%, where the matrix elements will decrease by this percentage on increasing k_f by that value. Also, the dependence of the second-order terms on variables of the center-of-mass quantum numbers N and L is found to lead to an uncertainty in these terms of about 10%. Dahlblom et al. (1964) found that the third-order terms are less than the second-order terms by about 20%, and also that the fourth-order terms are smaller, and so on. Our present calculations for the first- and second-order matrix elements are given in Tables VII and VIII.

In the present work, the Hartree-Fock equations are solved by an iteration procedure to obtain the binding energy per particle. The Hartree-Fock method is applied taking into account all the effects of tensor forces. The second-order terms from tensor forces are calculated and taken into account. The second-order terms from the pseudopotentials are also calculated and taken into account. Also, simple corrections due to both Coulomb energy and center-of-mass energy corrections are calculated and included.

The present work is applied to finite nuclei. In our calculations we used five harmonic-oscillator functions in the determination of each orbital. The present calculations have been applied for the two nuclei ^{16}O and ^{40}Ca for different values of the oscillator size parameter ν. The present calculated values of the binding energies per particle are listed in Table IX.

From the present calculations, it is clear that the unitary model operator approach is useful in discussing the effective interactions in nuclei. Also, many effects are quite large and must be taken into account, such as the

TABLE VII. First- and second-order matrix elements for the Tabakin potential (Yamaguchi)

State	nl	NL	First order $v^I_{12} - v_p$	$v_T^{OD}(Q/e)v_T^{OD}$	Second order $(v^I_{12} - v_p)(Q/e)(v^I_{12} - v_p)$
$^3S_1$	00	00	0.70	−9.62	−0.91
$^3S_1$	10	00	4.05	−10.11	−1.39
$^1S_0$	00	00	−7.04		−0.26
$^1S_0$	10	00	−4.96		−0.26
$^1P_1$	01	00	3.24		−1.85
$^3P_0$	01	00	−2.83		−0.35
$^3P_1$	01	00	3.26		−0.47
$^3P_2$	01	00	−1.51		
$^1D_2$	02	00	−1.23		
$^3D_1$	02	00	1.63		
$^3D_2$	02	00	−2.52		
$^3D_3$	02	00	0.12		

TABLE VIII. First- and second-order matrix elements for the Tabakin potential (Breit et al.)

State	nl	NL	First order $v^I_{12} - v_p$	$v_T^{OD}(Q/e)v_T^{OD}$	Second order $(v^I_{12} - v_p)(Q/e)(v^I_{12} - v_p)$
$^3S_1$	00	00	0.69	−9.29	−0.85
$^3S_1$	10	00	3.96	−10.01	−1.21
$^1S_0$	00	00	−6.88		−0.23
$^1S_0$	10	00	−4.84		−0.23
$^1P_1$	01	00	3.03		−1.72
$^3P_0$	01	00	−2.69		−0.32
$^3P_1$	01	00	3.08		−0.43
$^3P_2$	01	00	−1.31		
$^1D_2$	02	00	−0.92		
$^3D_1$	02	00	1.45		
$^3D_2$	02	00	−2.48		
$^3D_3$	02	00	0.11		

TABLE IX. Binding energy per particle

Nucleus	potential parameters used	Binding energy per particle (MeV) for different ν (fm) 1.48	1.76	2.16	2.38
^{16}O	Tabakin (Yamaguchi)	−6.63	−6.87	−4.42	−4.09
^{16}O	Tabakin (Breit et al.)	−6.36	−6.61	−4.06	−3.76
^{40}Ca	Tabakin (Yamaguchi)	−8.00	−8.45	−7.42	−6.17
^{40}Ca	Tabakin (Breit et al.)	−7.99	−8.50	−7.37	−6.14

second-order terms from both the tensor forces and the pseudopotentials. These effects, together with introducing pseudopotentials, help much to obtain reasonable agreement with the ground-state properties of finite closed-shell spherical nuclei.

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