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Spin-Orbit Doublet Separation in O^{17} Using Hard-Core Harmonic-Oscillator Wave Functions

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Calculations of the spin-orbit doublet separation in O^{17} are performed. It is assumed that, to a first approximation, the individual-particle potential experienced by each nucleon in the nucleus is given by the harmonic-oscillator potential. In this approximation the two-nucleon wave function for nucleons in the nucleus is separable in their relative and center-of-mass coordinates so that, taking into account only two-body interactions which depend on the relative coordinate, the K matrix elements are essentially functions of quantum numbers of relative motion only and of the relative space coordinate. The nucleus O^{17} is considered as consisting of the nucleus O^{16} as a core plus a neutron outside. The spin-orbit doublet separation is the difference in energy of O^{17} with the outside neutron in the states $J=\frac{5}{2}$ and $\frac{3}{2}$, and is evaluated in the approximation of taking interactions of the outside neutron with each of the sixteen core nucleons and neglecting interactions between nucleons in the core. Numerical calculations are done using only the spin-orbit part of the Gammel-Thaler potential, but treating it as a perturbation using hard-core harmonic-oscillator wave functions as the unperturbed wave functions. A value of 5.95 MeV is obtained for the spin-orbit splitting.

1. INTRODUCTION

THE problem of determining the two-nucleon interaction inside a nucleus has been a basic problem in nuclear physics. Largely, authors have worked with a phenomenological effective nucleon-nucleon interaction to predict nuclear properties (which also determine the parameters of the phenomenological effective two-nucleon interaction). Because of the presence of other nucleons in the nucleus, it seems that the effective two-nucleon interaction should be different from the free two-nucleon potential. However, it has not yet been possible to determine the effective nucleon-nucleon interaction[1] from basic principles. On the other hand, the work of Brueckner,[2] and of Bethe,[3] and others, on the nuclear many-body problem provides sufficient evidence that nuclear properties can be calculated by taking the two-nucleon interaction as that between two free nucleons, the latter being determined phenomenologically[4] from nucleon-nucleon scattering experiments.

The Brueckner-Bethe nuclear many-body theory has been worked out in terms of the reaction matrix derived from the free two-nucleon interaction, the reaction matrix being treated as the effective two-body interaction. Besides the difficulties involved in deriving the reaction matrix from the two-nucleon potential, the theory runs into a more formidable problem of calculating the self-consistent potential acting on an individual nucleon in the nucleus. Various approximations have been used to make the calculations tractable.

An alternative approach which has been used by several authors[5] is to assume the individual particle potential as given, viz., that each of the nucleons in the nucleus is moving under the influence of a common harmonic-oscillator potential and the two-body interaction as that of two free nucleons. The advantage of using the harmonic-oscillator potential is that, as shown by Talmi,[6] the wave function of the two nucleons in the nucleus is separable in their relative and center-of-mass coordinates. If the two-body interaction depends only on the relative coordinates, the calculations are now considerably simplified.

In this paper we have carried out a detailed calculation of the spin-orbit doublet separation in O^{17}, making use of the above model. The calculation of the spin-orbit interaction in nuclei has been previously reported

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[6] I. Talmi, Helv. Phys. Acta **25**, 185 (1952).

by several authors.[7] Many of these are Born-approximation calculations, some using only the tensor part of the two-nucleon interaction, resulting in the wrong sign and a much smaller value for the spin-orbit interaction in the nucleus. Various approximations have been made regarding the nuclear density in order to carry out a separation of the relative and center-of-mass coordinates. In the present article the "definite" model used is to regard, to a first approximation, the nucleus O^{17} as a system of seventeen independent nucleons moving in a common harmonic-oscillator potential. The eight protons and eight neutrons fill up the $1s$ and $1p$ configurations forming a core while the ninth (last) neutron goes into the $1d$ state so that O^{17} can be in the $J=\frac{3}{2}$ and $J=\frac{5}{2}$ state. The use of the harmonic-oscillator functions allows a calculation of the K matrix. To first order, the contributions of the central and tensor forces to the K matrix are identical in the $J=\frac{3}{2}$ and $J=\frac{5}{2}$ states, leaving only the contribution of the two-nucleon spin-orbit force. Thus the procedure involves adding up the spin-orbit contributions arising from the interaction of the d-state neutron with each of the sixteen nucleons in the core, assuming that the interaction between the core particles can be neglected, since it is common to both the $J=\frac{5}{2}$ and $J=\frac{3}{2}$ states. Finally the numerical calculation of the spin-orbit doublet separation in O^{17} is carried out by treating the spin-orbit interaction as a perturbation, using the hard-core wave functions as the unperturbed wave functions.

2. METHOD OF CALCULATION FOR O^{17}

In the case of O^{17}, the nucleus can be thought of as consisting of a neutron bound to a core which has no angular momentum. As a first approximation to the wave function of such a system, we assume that the wave function of the core is very nearly that of 16 independent particles. The justification of this is provided by Brueckner's work on nuclear matter. Following the lead of shell theory, we can assume that there are 2 neutrons and 2 protons in the lowest s state, and 6 neutrons and 6 protons in the second energy level, the first p state. We then express these orbitals in terms of harmonic-oscillator wave functions, since these are convenient to work with. In general, one would want to express the wave function of each orbital as a sum of harmonic oscillator functions with given l and m, but different n. However, in the present case, the assumption that there are 2 protons in the $1s$ state and 2 protons in each of the three ($m=\pm 1$, 0) $1p$ states, with no admixture of states of higher n, gives a charge density for O^{16} which agrees[8] well with experimental data, if $\sqrt{\nu}$ is chosen as 0.432 fm^{-1}. We therefore assume that this is true of O^{17} as well. Since all lower states are completely filled, the lowest available state for the 17th particle is either the $2s$ or $1d$ state. Experiment shows the ground state of O^{17} to have $J=\frac{5}{2}$, so the extra neutron would have to be in a $d_{5/2}$ state.

Taking into account only two-nucleon interactions, the Hamiltonian for O^{17} can be written in the form

$$H=\sum_{i=1}^{17}\frac{p_i^2}{2M}+\tfrac{1}{2}\sum_{i\neq j}v_N(|\mathbf{r}_i-\mathbf{r}_j|)\,, \tag{1}$$

where we have neglected the mass difference between the proton and the neutron, and the potential, v_N, is the two-nucleon potential, including central spin-orbit, and tensor forces, all with hard cores. The assumption that harmonic-oscillator orbitals can be used as a first approximation to describe the system is equivalent to doing a sort of perturbation theory, in which the Hamiltonian for the 17-nucleon system is modified to make part of it have the form of a harmonic oscillator. Thus, Eq. (1) is modified to read

$$H=H_0+V\,, \tag{2}$$

where

$$H_0=\sum_{i=1}^{17}[(1/2M)\mathbf{p}_i^2+\tfrac{1}{2}k|\mathbf{r}_i|^2] \tag{3a}$$

$$V=\tfrac{1}{2}\sum_{i\neq j}\{v_N(\mathbf{r}_{ij})-\tfrac{1}{2}(k/17)|\mathbf{r}_{ij}|^2\}\,. \tag{3b}$$

In writing Eq. (2) we have added and subtracted the harmonic oscillator terms

$$\tfrac{1}{2}k\sum_{i=1}^{N}|\mathbf{r}_i|^2=\tfrac{1}{4}(k/N)[\sum_{i\neq j}|\mathbf{r}_i-\mathbf{r}_j|^2+2(\sum_i \mathbf{r}_i)^2]$$

and assumed that the center of mass is fixed at the origin. The problem can now be treated by a "perturbation" theory. If we chose the unperturbed wave function well enough, the effect of V on the energy would be small, although it might change the form of the wave functions, e.g., by introducing correlation. Before one can use a perturbation series, or the related series expansions for the K matrix we must also include the hard-core part of V into the unperturbed Hamiltonian H_0. We rewrite

$$V=V_{\mathrm{HC}}+V_F\,, \tag{4a}$$

where

$$V_{\mathrm{HC}}=\sum_{i\neq j}v_{\mathrm{HC}};\ v_{\mathrm{HC}}(r_{ij})=\infty\,,\quad 0\leqslant r_{ij}\leqslant r_c \\ =0,\quad r_{ij}>r_c \tag{4b}$$

$$V_F=\tfrac{1}{2}\sum_{i\neq j}\{v_F(r_{ij})-\tfrac{1}{2}(k/17)|r_{ij}|^2\}\,, \tag{4c}$$

where v_F is the finite part of v_N.

We take the hard core into account in the following manner. The O^{16} particles are assumed to be in the $1s$ and $1p$ states ($nlm=000$; 010; and 01 ± 1), two neutrons

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and two protons being in each of these spatial states. The 17th nucleon is a neutron which is in the $1d$ state. We consider the particles two at a time, and express the products of the spatial states in terms of products of center-of-mass and relative states. The actual unperturbed relative states in each must take into account the hard core and are not the usual harmonic-oscillator wave functions. We therefore express[9] the relative states in terms of the hard-core solutions, but in each case the leading term is just the hard-core function with corresponding n, l, m; the coefficients of the functions n', l, m with $n'\neq n$ have been found to be extremely small, and can be neglected.

The next step is to calculate the corrected wave functions due to the potential V, as done by Brueckner.[2] These functions are, according to Brueckner's calculations, quite close to those for hard-core only, so it seems to be a justified procedure to use the hard-core functions to evaluate the matrix elements of the potential.

In order to find a first-order value for the spin-orbit splitting we need to calculate the difference in energy between the configuration having the extra neutron, particle "1," in the $d_{5/2}$ state as compared with the configuration with particle 1 in the $d_{3/2}$ state. Since the extra particle is the only one which has a different configuration in these two states, $J=\frac{5}{2}$ and $\frac{3}{2}$, in evaluating the difference in energy for these two states, we need not take into account the two-nucleon interactions among the core nucleons but include only the interaction of the d-state neutron with the core nucleons. The kinetic energy term is the same, since in both cases the outer neutron is in a d state. Thus, we calculate the difference in the potential energy terms, by evaluating only the K matrix elements involving particle No. 1, the d-state neutron:

$$\begin{aligned}(\Delta E)_{ls}&=\epsilon_{5/2}-\epsilon_{3/2}\\&=\langle 1;\mathrm{O}^{16}|K|1;\mathrm{O}^{16}\rangle_{5/2}-\langle 1;\mathrm{O}^{16}|K|1;\mathrm{O}^{16}\rangle_{3/2}.\end{aligned}\quad(5)$$

Each of these two K-matrix elements has the following form:

$$\langle 1;\mathrm{O}^{16}|K|1;\mathrm{O}^{16}\rangle=\sum_{c=2}^{17}(1,c|\mathcal{A}^{\dagger}K\mathcal{A}|1,c),\quad(6)$$

where $\mathcal{A}|i;j)=\frac{1}{2}\sqrt{2}[|i,j)-|j,i)]$, the numbers i and j stand for all the indices necessary to specify the state of each nucleon and c stands for a nucleon in the core. According to the foregoing procedure, we write the two-particle states $|1;c)$ as products of single-particle states, which will later be expressed in terms of relative states, with the hard core taken into account. We therefore write

$$\begin{aligned}|1;c)&=|1)\otimes|c)\\&=|n_1l_1s_1J_1M_1t_1(t_1)_3)\otimes|n_cl_cs_cJ_cM_ct_c(t_c)_3),\end{aligned}\quad(7)$$

where the relevant quantum numbers are specified as follows: For the extra neutron, we have $n_1=0$, $l_1=2$, $J_1=\frac{5}{2}$ or $\frac{3}{2}$ with $J_1\geqslant M_1\geqslant -J_1$. The sum is carried out for the 16 core particles which are in the quantum states $n_c=0$, $l_c=0$ ($J_c=\frac{1}{2}$, $M_c=\pm\frac{1}{2}$) and $l_c=1$ ($J_c=\frac{3}{2}$, $M_c=\pm\frac{3}{2},\pm\frac{1}{2}$; and $J_c=\frac{1}{2}$, $M_c=\pm\frac{1}{2}$), $(t_c)_3=\pm\frac{1}{2}$.

Since the Talmi procedure cannot be directly applied to the products of states in the l, s, J, M representation these must be expressed in terms of l, m, s, m_s states by means of Clebsch-Gordan coefficients.[10] That is,

$$\begin{aligned}|n_il_is_iJ_iM_it_it_{i3})=\sum_{m_s=-1/2,+1/2}&(l_is_im_im_{si}|J_iM_i)\\&\times|n_il_im_is_im_{si}t_it_{i3}),\end{aligned}\quad(8)$$

where $m_i=M_i-m_{si}$ for each m_{si}.

This should be done for particle one and for each of the core particles separately, before multiplying them and putting them into Eq. (6). However, we can avoid a lot of work by noting that the sum over core particles is carried over a complete shell. That is, each of the core functions $|l_cs_cJ_cM_c)$ can be expressed in terms of a linear combination of the $|l_cm_cs_cm_{sc})$, and vice versa, so that these two sets are simply two alternative basis sets for the same Hilbert space. Thus, we may regard the core particles as being in the sixteen states of type $|n_cl_cm_cs_c\times m_{sc}t_ct_{c3})$ with $n_c=0$, $l_c=0$ and 1 ($l_c\geqslant m_c\geqslant -l_c$); $s_c=\frac{1}{2}(m_{sc}=\pm\frac{1}{2})$ and $t_c=\frac{1}{2}(t_{c3}=\pm\frac{1}{2})$.

Using Eq. (8) for particle 1, we have from Eq. (6)

$$\begin{aligned}\langle 1;\mathrm{O}^{16}|K|1;\mathrm{O}^{16}\rangle=&\sum_{m_{s1}}\sum_{m_{s1}'}(l_1s_1m_1m_{s1}|J_1M_1)^*\\&\times(l_1s_1m_1'm_{s1}'|J_1M_1)\otimes\sum_{l_cm_c}\sum_{m_{sc}}\sum_{t_{c3}}(n_1l_1m_1s_1m_{s1}t_1t_{13};\\&\times n_cl_cm_cs_cm_{sc}t_ct_{c3}|\mathcal{A}^{\dagger}K\mathcal{A}|n_1l_1m_1's_1m_{s1}'t_1t_{13};\\&\times n_cl_cm_cs_ct_ct_{c3}).\end{aligned}\quad(9)$$

This expression can be put in a much simpler form by immediately carrying out the sums over m_{sc} and t_{c3}. To do this, we factor each of the states into a space part, spin part, and isospin part as follows:

$$|n_il_im_is_im_{si}t_it_{i3})=|n_il_im_i)|s_im_{si}\rangle|t_it_{i3}\rangle.\quad(10)$$

We first combine the spins of the two particles using Clebsch-Gordan coefficients. The reason for doing this is that for two-nucleon interaction the K matrix is diagonal in the total spin S. Thus, we write

$$|s_1m_{s1}\rangle|s_cm_{sc}\rangle=\sum_{S=0,1}(s_1s_cm_{s1}m_{sc}|SM)|s_1s_2SM\rangle.\quad(11)$$

We note that if $|s_1s_2SM\rangle$ is written in terms of the states $|s_1m_{s1}\rangle|s_cm_{sc}\rangle$, the result is the same as simply using the antisymmetrization operator for $S=0$ or the symmetrization operator for $S=1$. For instance, $|\frac{1}{2}\frac{1}{2}00\rangle=a|\frac{1}{2}\frac{1}{2};\frac{1}{2}\ -\frac{1}{2}\rangle$. Since the entire two-particle state is antisymmetric, the product of the space and isospin

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parts is symmetric for $S=0$, and antisymmetric for $S=1$.

Two distinct cases arise for the K matrix from Eq. (9).

(i) $m_{s1}=m_{s1}'=\pm\frac{1}{2}$: Neglecting the space and isospin part, we have

$$\sum_{m_{sc}} \langle s_1 m_{s1};\, s_c m_{sc}|K|s_1 m_{s1};\, s_c m_{sc}\rangle$$
$$\equiv \sum_{m_{sc}} \langle \tfrac{1}{2}\pm\tfrac{1}{2};\, \tfrac{1}{2}\, m_{sc}|K|\tfrac{1}{2}\pm\tfrac{1}{2};\, \tfrac{1}{2}\, m_{sc}\rangle$$
$$\equiv \langle \tfrac{1}{2}\pm\tfrac{1}{2};\, \tfrac{1}{2}\pm\tfrac{1}{2}|K|\tfrac{1}{2}\pm\tfrac{1}{2};\, \tfrac{1}{2}\pm\tfrac{1}{2}\rangle + \langle \tfrac{1}{2}\pm\tfrac{1}{2};\, \tfrac{1}{2}\mp\tfrac{1}{2}|K|\tfrac{1}{2}\pm\tfrac{1}{2};\, \tfrac{1}{2}\mp\tfrac{1}{2}\rangle.$$

Using Eq. (11), we obtain

$$\sum_{m_{sc}} \langle s_1 m_{s1};\, s_c m_{sc}|K|s_1 m_{s1};\, s_c m_{sc}\rangle$$
$$= \langle \tfrac{1}{2}\tfrac{1}{2}1\pm 1|K|\tfrac{1}{2}\tfrac{1}{2}1\pm 1\rangle + \{\tfrac{1}{2}\langle \tfrac{1}{2}\tfrac{1}{2}10|K|\tfrac{1}{2}\tfrac{1}{2}10\rangle + \tfrac{1}{2}\langle \tfrac{1}{2}\tfrac{1}{2}00|K|\tfrac{1}{2}\tfrac{1}{2}00\rangle \pm \tfrac{1}{2}\langle \tfrac{1}{2}\tfrac{1}{2}10|K|\tfrac{1}{2}\tfrac{1}{2}00\rangle$$
$$\pm \tfrac{1}{2}\langle \tfrac{1}{2}\tfrac{1}{2}00|K|\tfrac{1}{2}\tfrac{1}{2}10\rangle\} = K_1^{\pm1\,\pm1} + \tfrac{1}{2}K_1^{00} + \tfrac{1}{2}K_0^{00}, \quad (12)$$

where the upper sign is for $m_{s1}=+\frac{1}{2}$ and the lower sign is for $m_{s1}=-\frac{1}{2}$ and where the last two terms have been dropped since K is diagonal in S. The notation used is

$$\langle \tfrac{1}{2}\tfrac{1}{2}SM_S|K|\tfrac{1}{2}\tfrac{1}{2}S'M_{S'}\rangle = \delta_{SS'}K_S^{M_S M'_S}. \quad (13)$$

(ii) $m_{s1}=-m_{s1}'=\pm\frac{1}{2}$ (the spin-flip terms): In this case we have

$$\sum_{m_{sc}} \langle s_1 m_{s1};\, s_c m_{sc}|K|s_1 m_{s1}';\, s_c m_{sc}\rangle = \langle \tfrac{1}{2}\pm\tfrac{1}{2};\, \tfrac{1}{2}\pm\tfrac{1}{2}|K|\tfrac{1}{2}\mp\tfrac{1}{2};\, \tfrac{1}{2}\pm\tfrac{1}{2}\rangle$$
$$+\langle \tfrac{1}{2}\pm\tfrac{1}{2};\, \tfrac{1}{2}\mp\tfrac{1}{2}|K|\tfrac{1}{2}\mp\tfrac{1}{2};\, \tfrac{1}{2}\mp\tfrac{1}{2}\rangle = \{\tfrac{1}{2}\sqrt{2}\langle \tfrac{1}{2}\tfrac{1}{2}1\pm1|K|\tfrac{1}{2}\tfrac{1}{2}10\rangle \mp \tfrac{1}{2}\sqrt{2}\langle \tfrac{1}{2}\tfrac{1}{2}1\pm1|K|\tfrac{1}{2}\tfrac{1}{2}00\rangle\}$$
$$+\{\tfrac{1}{2}\sqrt{2}\langle \tfrac{1}{2}\tfrac{1}{2}10|K|\tfrac{1}{2}\tfrac{1}{2}1\mp1\rangle \pm \langle \tfrac{1}{2}\tfrac{1}{2}00|K|\tfrac{1}{2}\tfrac{1}{2}1\pm1\rangle\} = \tfrac{1}{2}\sqrt{2}\{K_1^{\pm1\,0} + K_1^{0\,\mp1}\}. \quad (14)$$

Exactly analogous manipulations are carried out in the case of isospin. Combining the isospin of the outer neutron with that of a core nucleon, we have

$$|t_1 t_{13}\rangle|t_c t_{c3}\rangle = \sum_{T=0,1} (t_1 t_c t_{13} t_{c3}|TT_3)|t_1 t_c T T_3\rangle, \quad (15)$$

where $t_{13}=-\frac{1}{2}$. From Eq. (15), and taking into account that the K matrix is diagonal in T and independent of T_3, we obtain

$$\sum_{t_{c3}} \langle t_1 t_{13};\, t_c t_{c3}|K_S^{M_S M'_S}|t_1 t_{13};\, t_c t_{c3}\rangle = \langle \tfrac{1}{2}-\tfrac{1}{2};\, \tfrac{1}{2}\tfrac{1}{2}|K_S^{M_S M'_S}|\tfrac{1}{2}-\tfrac{1}{2};\, \tfrac{1}{2}\tfrac{1}{2}\rangle$$
$$+\langle \tfrac{1}{2}-\tfrac{1}{2};\, \tfrac{1}{2}-\tfrac{1}{2}|K_S^{M_S M'_S}|\tfrac{1}{2}-\tfrac{1}{2};\, \tfrac{1}{2}-\tfrac{1}{2}\rangle = \tfrac{1}{2}\langle \tfrac{1}{2}\tfrac{1}{2}10|K_S^{M_S M'_S}|\tfrac{1}{2}\tfrac{1}{2}10\rangle + \tfrac{1}{2}\langle \tfrac{1}{2}\tfrac{1}{2}00|K_S^{M_S M'_S}|\tfrac{1}{2}\tfrac{1}{2}00\rangle$$
$$+\langle \tfrac{1}{2}\tfrac{1}{2}1-1|K_S^{M_S M'_S}|\tfrac{1}{2}\tfrac{1}{2}1-1\rangle = \tfrac{3}{2}K_{S(T=1)}^{M_S M'_S} + \tfrac{1}{2}K_{S(T=0)}^{M_S M'_S}. \quad (16)$$

Introducing the notation:

$$\langle SM_S TT_3|K|S'M_{S'}T'T'_3\rangle = \delta_{SS'}\delta_{TT'}\delta_{T_3T'_3}K_{ST}^{M_S M'_S} \quad (17)$$

and combining Eq. (12) with Eq. (16), we have the following.

(i) Non-spin-flip case, $m_{s1}=m_{s1}'=\pm\frac{1}{2}$:

$$\sum_{m_{sc}}\sum_{t_{c3}} \langle s_1 m_{s1} t_1 t_{31};\, s_c m_{sc} t_c t_{c3}|K|s_1 m_{s1} t_1 t_{13};\, s_c m_{sc} t_c t_{c3}\rangle$$
$$= (\tfrac{3}{2}K_{11}^{\pm1,\pm1} + \tfrac{1}{2}K_{10}^{\pm1,\pm1}) + \tfrac{1}{2}(\tfrac{3}{2}K_{11}^{00} + \tfrac{1}{2}K_{10}^{00}) + \tfrac{1}{2}(\tfrac{3}{2}K_{01}^{00} + \tfrac{1}{2}K_{00}^{00}). \quad (18)$$

(ii) Spin-flip case, $m_{s1}=-m_{s1}'=\pm\frac{1}{2}$:

$$\sum_{m_{sc}}\sum_{t_{c3}} \langle s_1 m_{s1} t_1 t_{13};\, s_c m_{sc} t_c t_{c3}|K|s_1 m_{s1}' t_1 t_{13};\, s_c m_{sc} t_c t_{c3}\rangle = \tfrac{1}{2}\sqrt{2}\{\tfrac{3}{2}(K_{11}^{\pm1,0} + K_{11}^{0,\mp1}) + \tfrac{1}{2}(K_{10}^{\pm1,0} + K_{10}^{0,\mp1})\}. \quad (19)$$

Using the fact that the entire state is antisymmetric for interchange of all indices, we group the terms of Eqs. (18) and (19) according to the symmetry of the associated space state. We thus obtain

$$\sum_{m_{sc}}\sum_{t_{c3}} \langle s_1 m_{s1} t_1 t_{13};\, s_c m_{sc} t_c t_{c3}|K|s_1 m_{s1}' t_1 t_{13};\, s_c m_{sc} t_c t_{c3}\rangle = \tfrac{1}{4}K_a^{\pm} + \tfrac{1}{4}K_s^{\pm} \quad \text{for} \quad m_{s1}=m_{s1}'$$
$$= (1/2\sqrt{2})(3K_a'^{\pm} + K_s'^{\pm}) \quad \text{for} \quad m_{s1}'=-m_{s1}, \quad (20)$$

where the subscripts s and a specify the symmetries of the spatial states, and where we define

$$K_a{}^{\pm}\equiv 3(2K_{11}{}^{\pm1,\pm1}+K_{11}{}^{00})+K_{00}{}^{00}, \tag{21a}$$

$$K_s{}^{\pm}\equiv (2K_{10}{}^{\pm1,\pm1}+K_{10}{}^{00})+3K_{01}{}^{00}, \tag{21b}$$

$$K_a{}^{f\pm}\equiv K_{11}{}^{\pm1\,0}+K_{11}{}^{0\,\mp1}, \tag{22a}$$

$$K_s{}^{f\pm}\equiv K_{10}{}^{\pm1\,0}+K_{10}{}^{0\,\mp1}. \tag{22b}$$

In terms of the above notation [Eq. (20)], we may rewrite Eq. (9) as follows:

$$\langle 1;O^{16}|K|1;O^{16}\rangle=\tfrac{1}{4}\sum_{m_{s1}}|(l_1s_1m_1m_{s1}|JM)|^2\{\sum_{l_cm_c}(n_1l_1m_1;\,n_cl_cm_c|\,\mathcal{A}^\dagger K_a{}^{\pm}\mathcal{A}+\mathcal{S}^\dagger K_s{}^{\pm}\mathcal{S}\,|n_1l_1m_1;\,n_cl_cm_c)\}+(1/2\sqrt{2})$$
$$\times\sum_{m_{s1}}(l_1s_1m_1'\,-m_{s1}|JM)(l_1s_1m_1m_{s1}|JM)^*\{\sum_{l_cm_c}(n_1l_1m_1;\,n_cl_cm_c|\,\mathcal{A}^\dagger 3K_a{}^{f\pm}\mathcal{A}+\mathcal{S}^\dagger K_s{}^{f\pm}\mathcal{S}\,|n_1l_1m_1';\,n_cl_cm_c)\}, \tag{23}$$

where

$$\mathcal{A}|nlm;\,n'l'm')\equiv\tfrac{1}{2}\sqrt{2}[|nlm)_1|n'l'm')_2-|n'l'm')_1|nlm)_2] \tag{24a}$$

$$\mathcal{S}|nlm;\,n'l'm')\equiv\tfrac{1}{2}\sqrt{2}[|nlm)_1|n'l'm')_2+|n'l'm')_1|nlm)_2], \tag{24b}$$

with

$$|nlm)_i=\phi_{nlm}(\mathbf{r}_i),\quad i=1,\,2.$$

Equation (23) is a sum of matrix elements of the two types

$$(n_1l_1m_1;\,n_cl_cm_c|\theta^\dagger K_\theta{}^{\pm}\theta|n_1l_1m_1;\,n_cl_cm_c) \tag{25a}$$

and

$$(n_1l_1m_1;\,n_cl_cm_c|\theta^\dagger K_\theta{}^{f\pm}\theta|n_1l_1m_1\pm1;\,n_cl_cm_c), \tag{25b}$$

where θ is one of the unitary operators a or s, and we have taken into account the fact that $m_1+m_{s1}=m_1'+m_{s1}'=M_1$, so that in the spin-flip matrix element (25b) we have $m_1'=m_1+m_{s1}-m_{s1}'=m_1\pm1$, since $m_{s1}=-m_{s1}'=\pm\frac{1}{2}$.

We wish to further diagonalize the K matrix, and to do this we use the property that the two-nucleon force is independent of the state of the two-particle center of mass, but depends strongly on the relative l and J of the two nucleons, as well as on their relative spatial wave function. However, it conserves the two-body total angular momentum J, and is independent of M_J. That is, the K matrix is diagonal in J and independent of M_J. We shall use these properties to reduce the number of matrix elements we need to calculate. The fact that the K matrix is independent of the relative M_J, which is equal to m_l+m_s, and of any of the quantum numbers of the center of mass, means that we may change the sign of all the angular momentum projections, m_1, m_c, M_S, and M'_S in the matrix elements (25a) and (25b) without affecting their value. Remembering that changing the superscript from $+$ to $-$ on K_a, K_s, $K_a{}^f$, and $K_s{}^f$ implies reversing the signs of M_S and M'_S, we write the following identity:

$$(n_1l_1m_1;\,n_cl_cm_c|\theta^\dagger\mathcal{K}_\theta{}^-\theta|n_1l_1m_1;\,n_cl_cm_c)=(n_1l_1\,-m_1;\,m_cl_c\,-m_c|\theta^\dagger\mathcal{K}_\theta{}^+\theta|n_1l_1\,-m_1;\,n_cl_c\,-m_c), \tag{26}$$

where $\mathcal{K}$ stands for K_a, K_s, $K_a{}^f$ or $K_s{}^f$. Equation (26) allows us to write Eq. (23) in the form (where $m_{s1}=\pm\frac{1}{2}$)

$$\langle 1;O^{16}|K|1;O^{16}\rangle=\tfrac{1}{4}\sum_{m_{s1}}\sum_{l_cm_c}|(l_1s_1m_1m_{s1}|JM)|^2$$
$$\times(n_1l_1\,\pm m_1;\,n_cl_c\,\pm m_c|\,\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}\,|n_1l_1\,\pm m_1;\,n_cl_c\,\pm m_c)+(1/2\sqrt{2})\sum_{m_{s1}}\sum_{l_cm_c}(l_1s_1m_1'\,-m_{s1}|JM)$$
$$\times(l_1s_1m_1m_{s1}|JM)^*(n_1l_1\,\pm m_1;\,n_cl_c\,\pm m_c|3\mathcal{A}^\dagger K_a{}^f\mathcal{A}+\mathcal{S}^\dagger K_s{}^f\mathcal{S}|n_1l_1\,\pm m_1';\,n_cl_c\,\pm m_c), \tag{27}$$

where the superscript $+$ on K is superfluous and is therefore dropped.

We now are in a position to express the symmetric and antisymmetric product functions $\theta|n_1l_1m_1;\,n_cl_cm_c)$ in terms of linear combinations of products of harmonic-oscillator states for the two-particle relative and center-of-mass quantum states $|nlm\rangle$ and $|NLM\rangle$, respectively. Thus we have

$$\theta|n_1l_1m_1;\,n_cl_cm_c)=\sum T_{\theta NLMnlm}{}^{n_1l_1m_1n_cl_cm_c}|NLM)|nlm\rangle, \tag{28}$$

where the T's are the Talmi coefficients,[6] which are functions of the quantum numbers $n_1l_1m_1$; $n_cl_cm_c$ and NLM; nlm, the summation is over possible values of N, L, M, n, l, and m; and θ stands for either "a" (antisymmetric) or "s" (symmetric). The symmetric and antisymmetric space states are defined in terms of the basic harmonic-oscillator states by Eqs. (24a) and (24b). The values of NLM and nlm are limited by the relations

$$m_1+m_c=M+m \tag{29}$$

$$(2n_1+l_1)+(2n_c+l_c)=(2N+L)+(2n+l). \quad (30)$$

It can be seen from parity considerations, or from direct calculation that for symmetric space states, l is always even, whereas for antisymmetric space states, l is always odd. As an example of two of these expansions, we have from Table IX (see Appendix A),

$$\mathcal{S}|022;01\ -1)=(1/\sqrt{20})|031)|000\rangle+(1/\sqrt{5})|111)|000\rangle+\tfrac{1}{2}|11\ -1)|022\rangle -(1/\sqrt{6})|011)|020\rangle-(1/\sqrt{3})|011)|100\rangle \quad (31a)$$

so that

$$T_{s013000}{}^{02201\ -1}=(1/\sqrt{20}),\quad T_{s011020}{}^{02201\ -1}=-(1/\sqrt{6}),\quad \text{etc.}$$

Similarly, from Table XII, we have

$$\mathcal{A}|022;01\ -1)=-(1/\sqrt{6})|020)|011\rangle-(1/\sqrt{3})|100)|011\rangle+\tfrac{1}{2}|022)|01\ -1\rangle +(1/\sqrt{20})|000)|031\rangle+(1/\sqrt{5})|000)|111\rangle. \quad (31b)$$

Using Eqs. (28) and (26), and taking into account that the K matrix is diagonal in the center of mass quantum numbers, we have for the matrix element (25a)

$$(n_1l_1\pm m_1;n_cl_c\pm m_c|\theta^\dagger K_\theta\theta|n_1l_1\pm m_1;n_cl_c\pm m_c)$$
$$=\sum_i\sum_k (T_{\theta N_kL_kM_kn_kl_km_k}{}^{n_1l_1m_1n_cl_cm_c})^* \times\langle n_kl_k\pm m_k|(N_kL_k\pm M_k|K_\theta|N_iL_i\pm M_i)|n_il_i\pm m_i\rangle T_{\theta N_iL_iM_in_il_im_i}{}^{n_1l_1m_1n_cl_cm_c} \quad (32a)$$
$$=\sum |T_{\theta NLMnlm}{}^{n_1l_1m_1n_cl_cm_c}|^2\langle nl\pm m|K_\theta|nl\pm m\rangle, \quad (32b)$$

subject to the restrictions (29) and (30). Thus, the non-spin-flip matrix elements depend only on the squares of the Talmi coefficients.

For the spin-flip terms, such as element (25b), we have, using Eqs. (26) and (28),

$$(n_1l_1\pm m_1;n_cl_c\pm m_c|\theta^\dagger K_\theta{}^f\theta|n_1l_1\pm m_1';n_cl_c\pm m_c)$$
$$=\sum_i\sum_k(T_{\theta N_kL_kM_kn_kl_km_k}{}^{n_1l_1m_1n_cl_cm_c})^* \times\langle n_kl_k\pm m_k)(N_kL_k\pm M_k|K_\theta{}^f|N_iL_i\pm M_i)|n_il_i\pm m_i\rangle T_{\theta N_iL_iM_in_il_im_i}{}^{n_1l_1m_1'n_cl_cm_c}$$
$$=\sum_i\sum_k(T_{\theta NLMn_kl_km_k}{}^{n_1l_1m_1n_cl_cm_c})^*(T_{\theta NLMn_il_im_i}{}^{n_1l_1m_1'n_cl_cm_c})\langle n_kl_k\pm m_k|K_\theta{}^f|n_il_i\pm m_i\rangle, \quad (33)$$

where the summations over i and k are carried out for which $|N_kL_k\pm M_k\rangle=|N_iL_i\pm M_i\rangle$. Taking into account that $m_1'=m_1\pm1$ [c.f., Eq. (25b)] and Eqs. (29) and (30), we have

$$M_i+m_i=m_c+m_1'=m_c+m_1\pm1=M_k+m_k\pm1 \quad (34a)$$
$$2(N_i+m_i)+(L_i+l_i)=2(n_1+n_c)+(l_1+l_c)=2(N_k+n_k)+(L_k+l_k), \quad (34b)$$

from which we have, for $(N_iL_iM_i)=(N_kL_kM_k)$, the results

$$m_i=m_k\pm1, \quad (35a)$$
$$2n_i+l_i=2n_k+l_k. \quad (35b)$$

Using Eqs. (35a) and (35b) in Eq. (33), we have

$$(n_1l_1\pm m_1;n_cl_c\pm m_c|\theta^\dagger K_\theta{}^f\theta|n_1l_1\pm m_1\pm1;n_cl_c\pm m_c)$$
$$=\sum_i\sum_k(T_{\theta NLMnlm}{}^{n_1l_1m_1n_cl_cm_c})^*(T_{\theta NLMn'l'm\pm1}{}^{n_1l_1m_1\pm1\ n_cl_cm_c})\langle nl\pm m|K_\theta{}^f|n'l'\pm m+1\rangle, \quad (36)$$

where $i=(NLM,nlm)$; $n'=n+k$; and $l'=l-2k$, to satisfy Eq. (35b). The index k is summed over all integers for which $l'\geqslant0$.

We note that in Eq. (27) these matrix elements are summed over all values of l_c and m_c. Therefore, we have arranged the Tables of Talmi coefficients so that these sums can be read off directly by simply adding the squares of the Talmi coefficients down each column, in case of no spin flip. In the spin-flip case, additional Tables are given for the coefficients required in Eq. (36). Thus, for instance, to find the matrix element sum: $\sum_{l_cm_c}(022;n_cl_cm_c|$

$\times \mathcal{S}^{+}K_s\mathcal{S}|022;\, n_cl_cm_c)$; we simply add the square of the coefficients of each relative term $|n_il_im_i\rangle$ down each column in Table IX to obtain

$$\sum_{l_cm_c}(022;\, n_cl_cm_c|\,\mathcal{S}^{\dagger}K_s\mathcal{S}\,|022;\, n_cl_cm_c)=(7/4)(K_s)_{000}+(5/4)(K_s)_{022}+\tfrac{1}{2}(K_s)_{021}+\tfrac{1}{6}(K_s)_{020}+\tfrac{1}{3}(K_s)_{100}, \tag{37}$$

where we have introduced the notation

$$(K_\theta)_{nlm}\equiv\langle nlm|K_\theta|nlm\rangle. \tag{38a}$$

If we introduce the notation

$$(K_\theta{}^f)_{nlm}\equiv\langle nlm|K_\theta{}^f|nl\; m\pm1\rangle, \tag{38b}$$

we can write the spin-flip terms in a similar compact form. We do not introduce a notation for $\langle nlm|K_\theta{}^f|n\pm1\; l\mp2\; m-1\rangle$ which can occur in Eq. (36), since we shall show in Appendix B that from angular momentum conservation these are zero. Using these notations we may go back and write Eq. (27) in terms of $(K_\theta)_{nlm}$ and $(K_\theta{}^f)_{nlm}$. Thus, we have, from Eqs. (27), (32b), and (36)

$$\begin{aligned}\langle 1;\mathrm{O}^{16}|K|1;\mathrm{O}^{16}\rangle=&\tfrac{1}{4}\sum_{m_{s1}=\pm1/2}|(l_1s_1m_1m_{s1}|JM)|^2\Big\{\sum_{l_cm_ci}|T_{aNLMnlm}{}^{n_1l_1m_1n_cl_cm_c}|^2(K_a)_{nl\,\pm m}\\&+\sum_{l_cm_c}\sum_i|T_{sNLMnlm}{}^{n_1l_1m_1n_cl_cm_c}|^2(K_s)_{nl\,\pm m}\Big\}+(1/2\sqrt{2})\sum_{m_{s1}=\pm1/2}(l_1s_1m_1\pm1\;-m_{s1}|JM)(l_1s_1m_1m_{s1}|JM)^*\\&\times\Big\{\sum_{l_cm_c}\sum_{i,k}(T_{sNLMnlm}{}^{n_1l_1m_1n_cl_cm_c})^*(T_{sNLMn'l'\;m\pm1}{}^{n_1l_1m_1\pm1\;n_cl_cm_c})(K_s{}^f)_{nl\,\pm m+1}\\&+3\sum_{l_cm_c}\sum_{i,k}(T_{aNLMnlm}{}^{n_1l_1m_1n_cl_cm_c})^*(T_{aNLMn'l'\;m\pm1}{}^{n_1l_1m_1\pm1\;n_cl_cm_c})(K_a{}^f)_{nl\,\pm m+1}\Big\}.\end{aligned} \tag{39}$$

We now recast Eq. (39) in a different form. Using a notation which divides K into a triplet part and a singlet part, we have from Eqs. (21a) for the non-spin-flip elements of K,

$$(K_s)_{nlm}=K_{(0)nlm}{}^1+3K_{(1)nlm}{}^0\quad\text{for even } l \tag{40a}$$

$$(K_a)_{nlm}=K_{(0)nlm}{}^0+3K_{(1)nlm}{}^1\quad\text{for odd } l, \tag{40b}$$

where

$$K_{(T)nlm}{}^{S=1}=2(K_{1T}{}^{11})_{nlm}+(K_{1T}{}^{00})_{nlm} \tag{41a}$$

$$K_{(T)nlm}{}^{S=0}=(K_{0T}{}^{00})_{nlm}, \tag{41b}$$

and a similar notation is used for the spin-flip elements.

We use this notation to write Eq. (39) in the compact form

$$\langle 1;\mathrm{O}^{16}|K|1;\mathrm{O}^{16}\rangle=\sum_{nl}\left\{\sum_{m=-l}^{l}(C_{nlm}{}^1K_{nlm}{}^1+C_{nlm}{}^0K_{nlm}{}^0)+\sum_{m=1}^{l}\frac{D_{nlm}}{[(l+m)(l-m+1)/2]^{1/2}}K_{nlm}{}^f\right\}, \tag{42}$$

where we have omitted the labels "T" since they can be inferred from the indices ls on K. The coefficients $C_{nlm}{}^s$, and D_{nlm} are combinations of Clebsch-Gordan coefficients and Talmi coefficients. From Eqs. (39) and (40) we have:

$$\begin{aligned}C_{nlm}{}^1=&\tfrac{3}{4}\sum_{m_{s1}=\pm1/2}|(l_1s_1m_1m_{s1}|JM)|^2\Big\{\sum_{l_cm_c}\sum_{NLM}|T_{aNL\,\pm Mnlm}{}^{n_1l_1\,\pm m_1n_cl_c\,\pm m_c}|^2\Big\}\quad\text{for odd } l\\=&\tfrac{1}{4}\sum_{m_{s1}=\pm1/2}(|l_1s_1m_1m_{s1}|JM)|^2\Big\{\sum_{l_cm_c}\sum_{NLM}|T_{sNL\,\pm Mnlm}{}^{n_1l_1\,\pm m_1n_cl_c\,\pm m_c}|^2\Big\}\quad\text{for even } l\end{aligned} \tag{43a}$$

$$\begin{aligned}C_{nlm}{}^0=&\tfrac{1}{3}C_{nlm}{}^1\quad\text{for odd } l\\=&3C_{nlm}\quad\text{for even } l\end{aligned} \tag{43b}$$

$$\begin{aligned}D_{nlm}=&\tfrac{3}{4}[(l+m)(l-m+1)]^{1/2}\sum_{m_{s1}=\pm1/2}(l_1s_1m_1\pm1\;m_{s1}|JM)(l_1s_1m_1m_{s1}|JM)^*\\&\times\sum_{l_cm_c}\sum_{NLM,k}(T_{sNLMnlm}{}^{n_1l_1\pm m_1n_cl_c\,\pm m_c})(T_{sNLM\;n+k\;l-2k\;m-1}{}^{n_1l_1\pm m_1+1n_cl_c\,\pm m_c})\quad\text{odd } l\\=&\tfrac{1}{4}[(l+m)(l-m+1)]^{1/2}\sum_{m_{s1}=\pm1/2}(l_1s_1m_1\pm1\;m_{s1}|JM)(l_1s_1m_1m_{s1}|JM)^*\\&\times\sum_{l_cm_c}\sum_{NLM,k}(T_{aNLMnlm}{}^{n_1l_1\,\pm m_1n_cl_c\,\pm m_c})(T_{aNLM\;n+k\;l-2k\;m-1}{}^{n_1l_1\pm m_1+1\;n_cl_c\,\pm m_c})\quad\text{even } l.\end{aligned}$$

Because of the relationship between the Talmi coefficients, the introduction of the radicals into the definition of the D's makes them rational fractions.

Our next step is to recombine the relative states $|nlm\rangle$ with the spin states implicit in the $K_{nlm}{}^s$ and $K_{nlm}{}^f$ to give states of the form $|nlSJM\rangle$. To do this, we use Clebsch-Gordan coefficients as follows:

$$|SM_S\rangle|nlm\rangle=\sum_J (lSmM_S|JM_J)|nlSJM_J\rangle. \quad (44)$$

Since K is diagonal in S and J, we can write

$$(K_{ST}{}^{M_SM'_S})_{nlm}=\sum_J (lSmM_S|JM_J)^* \times(lSmM'_S|JM'_J)k_{nl,J}{}^S, \quad (45)$$

where we have used the matrix elements

$$\langle nlSJM_J|K|nlS'J'M_J'\rangle=\delta_{SS'}\delta_{JJ'}k_{nl,J}{}^S. \quad (46)$$

These matrix elements are explicitly independent of M_J and M'_J.

We show in Appendix B that $K_{nlm}{}^s$ and $K_{nlm}{}^f$ can be expressed in the form

$$K_{nlm}{}^0=k_{nl,l}{}^0, \quad (47a)$$

$$K_{nlm}{}^1=\sum_{J=l-1}^{l+1}(A_{lJ}m+B_{lJ})k_{nl,J}{}^1, \quad (47b)$$

$$K_{nlm}{}^f=[(l+m)(l-m+1)/2]^{1/2}\sum_J A_{lJ}k_{nl,J}{}^1, \quad (47c)$$

where A_{lJ} and B_{lJ} are given in Table I.

TABLE I. Values of the coefficients A_{lJ} and B_{lJ}.

$J=$	$l+1$	l	$l-1$
$A_{lJ}=$	$\frac{2l+3}{(l+1)(2l+1)}$	$\frac{1}{l(l+1)}$	$\frac{2l-1}{l(2l+1)}$
$B_{lJ}=$	$\frac{2l+3}{2l+1}$	1	$\frac{2l-1}{2l+1}$

Incorporating the results of Eqs. (47a)–(47c) in Eq. (42) we have:

$$\langle 1;O^{16}|K|1;O^{16}\rangle=\sum_{nl}\{\mathcal{A}_{nl}{}^1(\sum_J B_{lJ}k_{nl,J}{}^1) +\mathcal{A}_{nl}{}^0k_{nl,J}{}^0+\mathcal{B}_{nl}(\sum_J A_{lJ}k_{nl,J}{}^1)\}, \quad (48)$$

where we define

$$\mathcal{A}_{nl}{}^1=\sum_{m=-l}^{l}C_{nlm}{}^1, \quad (49a)$$

$$\mathcal{A}_{nl}{}^0=\sum_m C_{nlm}{}^0, \quad (49b)$$

$$\mathcal{B}_{nl}=\sum_m (mC_{nlm}{}^1+D_{nlm}). \quad (49c)$$

In Sec. 4 we obtain the explicit expressions in the form of Eq. (48), for particle 1 in states $J=\frac{5}{2}$, $M=\frac{1}{2},\frac{3}{2},\frac{5}{2}$, and find, of course that they are identical (although the $C_{nlm}{}^s$ are *not* identical for the various M values). Then, we obtain similar expressions for the case $J=\frac{3}{2}$, $M=\frac{1}{2},\frac{3}{2}$. Finally, we subtract these, and obtain

$$\Delta\epsilon=\langle 1;O^{16}|K|1;O^{16}\rangle_{J=5/2}-\langle 1;O^{16}|K|1;O^{16}\rangle_{J=3/2} =\sum_{nl}\{(\Delta\mathcal{A})_{nl}{}^1(\sum_J B_{lJ}k_{nl,J}{}^1)+(\Delta\mathcal{A})_{nl}{}^0k_{nl,J}{}^0 +(\Delta\mathcal{B})_{nl}(\sum_J A_{lJ}k_{nl,J}{}^1)\}, \quad (50)$$

where

$$(\Delta\mathcal{A})_{nl}{}^S=(\mathcal{A}_{nl}{}^S)_{J=5/2}-(\mathcal{A}_{nl}{}^S)_{J=3/2} \quad (51)$$

As we will show in Sec. 4E that for O^{17}, $(\Delta\mathcal{A})_{nl}{}^S=0$, we finally obtain

$$\Delta\epsilon=\sum_{nl}\Delta\mathcal{B}_{nl}(\sum_J A_{lJ}k_{nl,J}{}^1). \quad (52)$$

We have now proceeded as far as possible without taking account of a particular form for the nucleon two-body force. The k matrix is expanded in terms of the potential V_F [cf., Eq. (4c)] as follows:

$$k_{nl,J}{}^S=(V_F)_{nl,J}{}^S+\sum_{n'l'}\frac{|\langle nlSJ|V_F|n'l'SJ\rangle|^2}{\epsilon_{n'l'}-\epsilon_{nl}}+\cdots. \quad (53)$$

This expansion takes into account the perturbation of the two-nucleon hard-core wave function by the potential V_F. From Eq. (4c), we have for V_F the following:

$$V_F(1,c)=v_F(1,c)-\tfrac{1}{2}k'|r_{1c}|^2, \quad (54)$$

where $v_F(1,c)$ is the finite part of the two-nucleon interaction.

The two nucleon potential v_F given by Gammel and Thaler[4] contains a central part, a spin-orbit part, and a tensor part, which operate outside a hard-core of radius 0.4 fm. Thus, we may write

$$V_F(1,2)=V_{GT}{}^C(r_{12})-\tfrac{1}{2}k'r_{12}{}^2+V_{GT}{}^{ls}(r_{12})\mathbf{L}_{12}\cdot\mathbf{S} +V_{GT}{}^T(r_{12})S_{12} \quad (55)$$

$$\langle nlSJM|V_F|n'l'S'J'M'\rangle =\{\langle nl|(V_{GT}{}^C(r)-\tfrac{1}{2}k'r^2)|n'l'\rangle\delta_{ll'} +\langle nl|V_{GT}{}^{ls}|n'l\rangle\mathcal{L}_{lJ}\delta_{s1}\delta_{ll'} +\langle nl|V_{GT}{}^T|n'l'\rangle\mathcal{T}_{ll'J}\delta_{s1}\}\delta_{JJ'}\delta_{SS'}\delta_{MM'}, \quad (56)$$

where $V_{GT}{}^C(r)$, $V_{GT}{}^{ls}(r)$, and $V_{GT}{}^T(r)$ are the radial parts belonging to the central, spin-orbit, and tensor forces given by Gammel-Thaler.[4] The matrix elements of the spin-orbit and tensor operators are

$$\langle SlJM|\mathbf{L}\cdot\mathbf{S}|S'l'J'M'\rangle=\delta_{MM'}\delta_{JJ'}\delta_{SS'}\delta_{ll'}\delta_{S1}\mathcal{L}_{lJ} \quad (57a)$$

$$\langle SlJM|S_{12}|S'l'J'M'\rangle=\delta_{MM'}\delta_{JJ'}\delta_{SS'}\delta_{S1}\mathcal{T}_{ll'J}, \quad (57b)$$

where the $\mathcal{L}_{lJ}$ and $\mathcal{T}_{lJ}$ are given in the Table II.

TABLE II. Matrix elements of the spin-orbit and tensor operators.

$l'=$	l	l	l	$l+2$	$l-2$
$J=$	$l+1$	l	$l-1$	$l+1$	$l-1$
$\mathcal{L}_{lJ}=$	l	0	$-(l+1)$	0	0
$\mathcal{T}_{ll'J}=$	$\dfrac{-2l}{2l+3}$	2	$\dfrac{2(l+1)}{2l-1}$	$\dfrac{6[(l+1)(l+2)]^{1/2}}{l+3}$	$\dfrac{6[l(l-1)]^{1/2}}{2l-1}$

3. FIRST-ORDER ENERGY DIFFERENCE

We now specialize the calculations to first order. Using Eqs. (52), (53), and (55), we have

$$\begin{aligned}\Delta\epsilon&=\sum_{nl}(\Delta\mathcal{B})_{nl}\sum_J A_{lJ}\langle nl1JM|V_F|nl1JM\rangle\\&=\sum_{nl}(\Delta\mathcal{B})_{nl}\sum_J A_{lJ}\{(V_{GT}{}^C)_{nl}-\tfrac12(k'r^2)_{nl}\\&\qquad+\mathcal{L}_{lJ}(V_{GT}{}^{ls})_{nl}+\mathcal{T}_{ll,J}(V_{GT}{}^T)_{nl}\}\\&=\sum_{nl}(\Delta\mathcal{B})_{nl}[2-1/l(l+1)](V_{GT}{}^{ls})_{nl},\end{aligned}\qquad(58)$$

where we have used the following equations which are easily proved using Tables II and I:

$$\sum_J A_{lJ}=\sum_J A_{lJ}\mathcal{T}_{ll,J}=\sum_J B_{lJ}\mathcal{T}_{llJ}=0$$

$$\sum_J A_{lJ}\mathcal{L}_{lJ}=2-1/l(l+1)\qquad(59)$$

$$\sum_J B_{lJ}=3;\quad \sum_J B_{lJ}\mathcal{L}_{lJ}=1.$$

We have also used the notation:

$$\begin{aligned}(V_{GT}{}^{ls})_{nl}&\equiv\langle nl|V_{GT}{}^{ls}(r)|nl\rangle\\&=\int_{r_c}^{\infty}\psi_{nl}{}^*(r)V_{GT}{}^{ls}(r)\psi_{nl}(r)r^2dr,\end{aligned}\qquad(60)$$

where $\psi_{nl}(r)$ are the wave functions for the relative motion of two particles in a harmonic oscillator, with a hard-core potential.

4. NUMERICAL CALCULATIONS

A. Case $J_1=\frac52$, $M_1=\frac32$

For this case, the outer neutron is in the state $J_1=\frac52$ and $M_1=\frac32$, and Eq. (8) for the state of the extra neutron becomes:

$$\begin{aligned}|n_1l_1s_1J_1M_1t_1t_{13})&=|02\tfrac12\tfrac52\tfrac32\tfrac12\,-\tfrac12)\\&=\sum_{m_{s1}=-1/2}^{1/2}(2\tfrac12 m_1m_{s1}|\tfrac52\tfrac32)|n_1l_1m_1s_1m_{s1}t_1t_{13})\\&=\sqrt{\tfrac45}|021\tfrac12\tfrac12\tfrac12\,-\tfrac12)+\sqrt{\tfrac15}|022\tfrac12\,-\tfrac12\tfrac12\,-\tfrac12).\end{aligned}\qquad(61)$$

Carrying out all the manipulations, we obtain, for Eq. (27), the expression:

$$\begin{aligned}\langle 1;O^{16}|K|1;O^{16}\rangle&=\tfrac15\sum_{l_cm_c}(021;n_cl_cm_c|\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}\\&\quad\times|021;n_cl_cm_c)+\frac{1}{20}\sum_{l_cm_c}(02\,-2;n_cl_cm_c|\\&\quad\times\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}|02\,-2;n_cl_cm_c)\\&\quad+\frac{2\sqrt2}{10}\sum_{l_cm_c}(022;n_cl_cm_c|3\mathcal{A}^\dagger K_a{}^f\mathcal{A}+\mathcal{S}^\dagger K_s{}^f\mathcal{S}\\&\qquad\times|021;n_cl_cm_c),\end{aligned}\qquad(62)$$

where the -2 in the second term comes about through the use of Eq. (26).

Using the tables of Talmi coefficients (Appendix A, Table X), we can write for Eqs. (32) and (33)

$$\begin{aligned}&\sum_{l_cm_c}(021;n_cl_cm_c|\mathcal{S}^\dagger K_s\mathcal{S}|021;n_cl_cm_c)\\&=(7/4)(K_s)_{000}+\tfrac12(K_s)_{022}+\tfrac34(K_s)_{021}+(5/12)(K_s)_{020}\\&\qquad+\tfrac14(K_s)_{02\,-1}+\tfrac13(K_s)_{100}.\end{aligned}\qquad(63a)$$

From Table IX, changing the signs of all m's

$$\begin{aligned}&\sum_{l_cm_c}(02\,-2;n_cl_cm_c|\mathcal{S}^\dagger K_s\mathcal{S}|02\,-2;n_cl_cm_c)\\&=(7/4)(K_s)_{000}+(5/4)(K_s)_{02\,-2}+\tfrac12(K_s)_{02\,-1}\\&\qquad+\tfrac16(K_s)_{020}+\tfrac13(K_s)_{100}.\end{aligned}\qquad(63b)$$

Similarly

$$\begin{aligned}&\sum_{l_cm_c}(021;n_cl_cm_c|\mathcal{A}^\dagger K_a\mathcal{A}|021;n_cl_cm_c)\\&=(5/4)(K_a)_{011}+(5/4)(K_a)_{010}+\tfrac14(K_a)_{01\,-1}\\&\qquad+\tfrac12(K_a)_{032}+\tfrac25(K_a)_{031}+(3/20)(K_a)_{030}\\&\qquad+\tfrac{1}{10}(K_a)_{111}+\tfrac{1}{10}(K_a)_{110},\end{aligned}\qquad(64a)$$

$$\begin{aligned}&\sum_{l_cm_c}(02\,-2;n_cl_cm_c|\mathcal{A}^\dagger K_a\mathcal{A}|02\,-1;n_cl_cm_c)\\&=(9/4)(K_a)_{01\,-1}+\tfrac14(K_a)_{010}+\tfrac14(K_a)_{011}+\tfrac34(K_a)_{03\,-3}\\&\qquad+\tfrac14(K_a)_{03\,-2}+(1/20)(K_a)_{03\,-1}+\tfrac15(K_a)_{11\,-1},\end{aligned}\qquad(64b)$$

$$\begin{aligned}&\sum_{l_cm_c}(022;n_cl_cm_c|\mathcal{S}^\dagger K_s{}^f\mathcal{S}|021;n_cl_cm_c)\\&\qquad=\tfrac34(K_s{}^f)_{022}+(3/2\sqrt6)(K_s{}^f)_{032},\end{aligned}\qquad(64c)$$

$$\begin{aligned}&\sum_{l_cm_c}(022;n_cl_cm_c|\mathcal{S}^\dagger K_s{}^f\mathcal{S}|021;n_cl_cm_c)\\&=\sqrt2(K_a{}^f)_{011}+(3/2\sqrt6)(K_a{}^f)_{032}+(1/\sqrt{10})(K_a{}^f)_{032}\\&\qquad+(3/20\sqrt3)(K_a{}^f)_{031}+(1/5\sqrt2)(K_a{}^f)_{111}.\end{aligned}\qquad(64d)$$

Putting Eqs. (63) into Eq. (62) yields the equation corresponding to Eq. (39):

$$\langle 1;O^{16}|K|1;O^{16}\rangle=(7/18)(K_s)_{000}+\tfrac{1}{12}(K_s)_{100}+(21/80)(K_a)_{011}+(21/80)(K_a)_{010}+(13/80)(K_a)_{01\,-1}$$
$$+(1/50)(K_a)_{111}+(1/50)(K_a)_{110}+(1/100)(K_a)_{11\,-1}+\tfrac{1}{10}(K_s)_{022}+(3/20)(K_s)_{021}+(11/120)(K_s)_{020}$$
$$+(3/40)(K_s)_{02\,-1}+(1/18)(K_s)_{02\,-2}+(3/80)(K_a)_{03\,-3}+(1/80)(K_a)_{03\,-2}+(1/400)(K_a)_{03\,-1}+(3/100)(K_a)_{030}$$
$$+(2/25)(K_a)_{031}+\tfrac{1}{10}(K_a)_{032}+(6/5)(K_a{}^f)_{110}+(3/25)(K_a{}^f)_{111}+(3/10\sqrt{2})(K_s{}^f)_{022}+(3/10\sqrt{3})(K_s{}^f)_{021}$$
$$+(9/10\sqrt{3})(K_a{}^f)_{033}+(3/5\sqrt{5})(K_a{}^f)_{032}+(9/50\sqrt{6})(K_a{}^f)_{031}. \quad (65)$$

Using Eqs. (21a) and (21b) this can be written in the form given in Eq. (42). The coefficients $C_{nlm}{}^S$ and D_{nlm} are listed in Table III.

Combining the $|nlm\rangle$ states with the $|SM_S\rangle$ states gives Eq. (48). From Table III (a, b, and c) and the definitions (49a)–(49c), we have for $\mathcal{A}_{nl}{}^S$ and $\mathcal{B}_{nl}$ the values in Table IV.

B. Case $J_1=\frac{5}{2}$, $M_1=\frac{1}{2}$

In this case, the outer neutron is in the state $J_1=\frac{5}{2}$, $M_1=\frac{1}{2}$ and Eq. (8) for the state of the extra neutron becomes

$$|n_1l_1s_1J_1M_1t_1t_{13})=\sqrt{\tfrac{3}{5}}|020\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\,-\tfrac{1}{2})+\sqrt{\tfrac{2}{5}}|021\tfrac{1}{2}\,-\tfrac{1}{2}\tfrac{1}{2}\,-\tfrac{1}{2}). \quad (66)$$

This results in the following form for Eq. (27):

$$\langle 1;O^{16}|K|1;O^{16}\rangle=(3/20)\sum_{l_cm_c}(020;n_cl_cm_c|\times\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}|020;n_cl_cm_c)$$
$$+\tfrac{1}{10}\sum_{l_cm_c}(02\,-1;n_cl_cm_c|\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}\times|02\,-1;n_cl_cm_c)+2\sqrt{3}\sum_{l_cm_c}(021;n_cl_cm_c|$$
$$\times 3\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}|020;n_cl_cm_c). \quad (67)$$

Using the Tables of Talmi coefficients to express the sums in Eq. (67) and Eqs. (23b) and (23c) yields the interaction in the form of Eq. (42). Although all the C's are different, their sums are the same, and whereas even $\sum_m D$ is different in the two cases, the quantity $\mathcal{B}_{nl}=\sum_m D+\sum_m mC$ is identical with the previous case. Thus, this calculation acts as a check of the figures obtained previously, and confirms the statement that the same energy expression suffices for both $M_1=\frac{3}{2}$ and $M_1=\frac{1}{2}$.

C. Case $J_1=\frac{3}{2}$, $M_1=\frac{3}{2}$

The same procedure is used to find the interaction for the case that the neutron is in the state $J_1=\frac{3}{2}$, $M_1=\frac{3}{2}$:

$$|n_1l_1s_1J_1M_1t_1t_{13})=\sqrt{\tfrac{4}{5}}|022\tfrac{1}{2}\,-\tfrac{1}{2}\tfrac{1}{2}\,-\tfrac{1}{2})-\sqrt{\tfrac{1}{5}}|021\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\,-\tfrac{1}{2}). \quad (68)$$

Thus, we have

$$\langle 1;O^{16}|K|1;O^{16}\rangle=\tfrac{1}{5}\sum_{l_cm_c}(02\,-2;n_cl_cm_c|\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}\times|02\,-2;n_cl_cm_c)+\frac{1}{20}\sum_{l_cm_c}(021;n_cl_cm_c|$$
$$\times\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}|021;n_cl_cm_c)-\frac{\sqrt{2}}{5}\sum_{l_cm_c}(022;n_cl_cm_c|$$
$$\times 3\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}|021;n_cl_cm_c). \quad (69)$$

The matrix elements in Eq. (69) are the same as those in Eq. (62); the case $J_1=\frac{5}{2}$, $M_1=\frac{3}{2}$, but they have different coefficients. They are given in Eqs. (63a)–(64d). Using these in Eq. (69) and using Eqs. (21a) and (21b)

TABLE III. Values of $C_{nlm}{}^S$ and D_{nlm} for $J_1=\frac{5}{2}$, $M_1=\frac{3}{2}$.

(a) $C_{nlm}{}^1$	$m=3$	2	1	0	-1	-2	-3	$\sum_m C_{nlm}{}^1$	$\sum_m mC_{nlm}{}^1$
$nl=00$	...	...	...	7/16	...	...	...	7/16	0
01	...	...	63/80	63/80	39/80	...	...	33/16	3/10
02	...	1/10	3/20	11/120	3/40	1/16	...	23/48	3/20
03	0	3/10	6/25	9/100	3/400	3/80	9/80	63/80	21/50
10	...	...	...	1/12	...	...	...	1/12	0
11	...	...	3/50	3/50	3/100	...	...	3/20	3/10

(b) $C_{nlm}{}^0$	$m=3$	2	1	0	-1	-2	-3	$\sum_m C_{nlm}{}^0$
$nl=00$	...	...	...	21/16	...	...	...	21/16
01	...	...	21/80	21/80	13/80	...	...	11/16
02	...	3/10	9/20	11/40	9/40	3/16	...	23/16
03	0	1/10	2/25	3/100	1/400	1/80	3/80	21/80
10	...	...	...	1/4	...	...	...	1/4
11	...	...	1/50	1/50	1/100	...	...	1/20

(c) D_{nlm}	$m=3$	2	1	$\sum_m D_{nlm}$	$\mathcal{B}_{nl}$
$nl=01$	...	...	6/5	6/5	3/2
02	...	3/10	3/10	3/5	3/4
03	9/10	6/10	9/50	42/25	21/10
11	...	...	6/50	6/50	3/20

TABLE IV. $\mathcal{A}_{nl}{}^{S}$ and $\mathcal{B}_{nl}$ for $J_1=\frac{5}{2}$, $M_1=\frac{3}{2}$.

nl	$\mathcal{A}_{nl}$	$\mathcal{A}_{nl}{}^{0}$	$\mathcal{B}_{nl}$
00	7/16	21/16	0
01	33/16	11/16	3/2
02	23/48	23/16	3/4
03	63/80	21/80	21/10
10	1/12	1/4	0
11	3/20	1/20	3/20

yields the interaction in the form of Eq. (42) with the coefficients given in Table V (a, b, and c).

The energy is given by the same formula [Eq. (48)] in terms of the $\mathcal{A}$'s and $\mathcal{B}$'s given by Table V (a, b, and c).

D. Case $J_1=\frac{3}{2}$, $M_1=\frac{1}{2}$

In this case the neutron wave function is

$$|n_1l_1s_1J_1M_1t_1t_{13})=\sqrt{\tfrac{3}{5}}\,|021\tfrac{1}{2}\,-\tfrac{1}{2}\tfrac{1}{2}\,-\tfrac{1}{2})-\sqrt{\tfrac{1}{5}}\,|020\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\,-\tfrac{1}{2}),$$

and we have

$$\langle 1;\mathrm{O}^{16}|K|1;\mathrm{O}^{16}\rangle=\frac{3}{20}\sum_{l_cm_c}(02\,-1;n_cl_cm_c|\times\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}|02\,-1;n_cl_cm_c)+\tfrac{1}{10}\sum_{l_cm_c}(020;n_cl_cm_c|\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}|020;n_cl_cm_c)-\frac{\surd 3}{5}\sum_{l_cm_c}(021;n_cl_cm_c|3\mathcal{A}^\dagger K_a\mathcal{A}+\mathcal{S}^\dagger K_s\mathcal{S}\times|020;n_cl_cm_c). \quad (70)$$

It can be verified that the $\mathcal{A}$'s and $\mathcal{B}$'s are the same in this case as in the case $J_1=\frac{3}{2}$, $M_1=\frac{3}{2}$ (although the C's and D's are quite different in the two cases).

E. Energy Difference $\Delta\varepsilon$ to the First Order

Since the $\mathcal{A}$ coefficients are the same in both the $J_1=\frac{5}{2}$ and the $J_1=\frac{3}{2}$ case (see Tables IV and V, the $\mathcal{A}$ coefficients in the difference expression cancel out, leaving only the $\mathcal{B}$ coefficients for the final expression. Thus, the difference in energy of the extra neutron between the $J_1=\frac{5}{2}$ and $J_1=\frac{3}{2}$ case, i.e., the spin-orbit splitting is given by an expression of the form

$$\Delta\epsilon=\sum_{nl}(\Delta\mathcal{B})_{nl}(\sum_J A_{lJ}k_{nl,J}{}^1). \quad (71)$$

To evaluate the first-order energy splitting, we use V for K in Eq (71). The matrix elements of V are given in Eq. (55) and Table II. Using these, we obtain Eq. (58), namely,

$$\Delta\epsilon=\sum_{nl}(\Delta\mathcal{B})_{nl}[2-1/l(l+1)](V_{GT}{}^{ls})_{nl}, \quad (72)$$

where

$$(V_{GT}{}^{ls})_{nl}=\int_{c r}^{\infty}\psi_{nl}{}^*(r)V_{GT}{}^{ls}(l,r)\psi_{nl}(r)r^2dr. \quad (73)$$

The coefficients of $(V_{GT}{}^{ls})_{nl}$ can be obtained by subtracting the results for the $\mathcal{B}_{nl}$ for $J_1=\frac{3}{2}$ from those for $J_1=\frac{5}{2}$, and multiplying by $[2-1/l(l+1)]$ as indicated in Table VI.

Our final expression for the first-order energy is

$$\Delta\epsilon=(45/8)(V_{GT}{}^{ls})_{01}+(55/16)(V_{GT}{}^{ls})_{02}+(161/16)(V_{GT}{}^{ls})_{03}+(9/16)(V_{GT}{}^{ls})_{11}. \quad (74)$$

The Gammel-Thaler[4] spin-orbit force is given by

$$\begin{aligned}V_{GT}{}^{ls}(l,r)&=-(5000\text{ MeV})e^{-3.7r}/3.7r \quad \text{for even } l\\&=-(7315\text{ MeV})e^{-3.7r}/3.7r \quad \text{for odd } l,\end{aligned} \quad (75)$$

where r is the internucleon distance in fm.

The value of $\Delta\epsilon$ using Eqs. (74) and (75) with hard-core wave functions has been evaluated in an earlier paper.[9] The result obtained is as follows:

$$\Delta\epsilon=E_{5/2}-E_{3/2}=(45/8)(-0.752)+(55/16)(-0.064)+(161/16)(-0.0044)+(9/16)(-2.38)=-5.95\text{ MeV}. \quad (76)$$

TABLE V. Values of $C_{nlm}{}^{S}$ and D_{nlm} for $J_1=\frac{3}{2}$, $M_1=\frac{3}{2}$.

(a) $C_{nlm}{}^1$	$m=3$	2	1	0	-1	-2	-3	$\mathcal{A}_{nl}{}^1$
$nl=00$	···	···	···	7/16	···	···	···	7/16
01	···	···	27/80	27/80	111/80	···	···	33/16
02	···	1/40	3/80	13/240	9/80	1/4	···	23/48
03	0	3/40	3/50	9/400	3/100	3/20	9/20	63/80
10	···	···	···	1/12	···	···	···	1/12
11	···	···	3/200	3/200	6/50	···	···	3/20

(b) $C_{nlm}{}^0$	$m=3$	2	1	0	-1	-2	-3	$\mathcal{A}_{nl}{}^0$
$nl=00$	···	···	···	21/16	···	···	···	21/16
01	···	···	9/80	9/80	37/80	···	···	11/16
02	···	3/40	9/80	13/80	27/80	3/4	···	23/16
03	0	1/40	1/50	3/400	1/100	1/20	3/20	21/80
10	···	···	···	1/4	···	···	···	1/4
11	···	···	1/200	1/200	1/25	···	···	1/20

(c) D_{nlm}	$m=3$	2	1	Sum	$\mathcal{B}_{nl}$
$nl=01$	···	···	$-6/5$	$-6/5$	$-9/4$
02	···	$-3/10$	$-3/10$	$-3/5$	$-9/8$
03	$-9/10$	$-3/5$	$-9/50$	$-42/25$	$-63/20$
11	···	···	$-3/25$	$-3/25$	$-9/40$

TABLE VI. Values of $\Delta\mathcal{B}_{nl}$.

nl	$\mathcal{B}_{nl}(J=\frac{5}{2})$	$\mathcal{B}_{nl}(J=\frac{3}{2})$	$(\Delta\mathcal{B})_{nl}$	$\Delta\mathcal{B}[2-1/l(l+1)]$
01	3/2	− 9/4	15/4	45/8
02	3/4	− 9/8	15/8	55/16
03	21/10	−63/20	21/4	161/16
11	3/20	− 9/40	3/8	9/16

5. SUMMARY

Assuming that as a first approximation, the individual-particle potential experienced by each nucleon in the nucleus is given by the harmonic-oscillator potential, the Hamiltonian for the nucleus (taking into account only two-nucleon interaction) is written as a sum of an unperturbed Hamiltonian corresponding to the harmonic-oscillator Hamiltonian and all the two-nucleon interactions minus the harmonic-oscillator potential [Eq. (2)]. We consider the problem of spin-orbit interaction in O^{17}. The nucleus O^{17} can be considered as consisting of O^{16} core plus an (extra) neutron outside; the particles in O^{16} fill up the $1s$ and $1p$ states ($nlm=000$; 010; and 01 ± 1 with two neutrons and two protons being in each of these spatial states) with the last neutron occupying the $1d$ state with $J=\frac{5}{2}$ or $\frac{3}{2}$. In order to determine the spin-orbit splitting it is necessary to calculate the difference in energy between the configurations having the extra neutron in the states $d_{5/2}$ and $d_{3/2}$. In calculating this difference it is assumed that the core being common to both the configurations, the two-nucleon interactions among the core particles can be neglected. Thus we need to evaluate the diagonal elements of the K matrix for the nuclear wave functions which are the two-particle states involving the extra neutron and each of the nucleons in the core [Eqs. (5) and (10)] for the two cases when the extra neutron is in the $d_{5/2}$ state and $d_{3/2}$ state. The difference $K(d_{5/2})-K(d_{3/2})$ determines the spin-orbit splitting [Eq. (5)]. It is advantageous to express the two-particle oscillator wave function $|n_1l_1m_1n_2l_2m_2\rangle$ in terms of the linear combination $\sum_i T_{n_il_im_iN_iL_iM_i}{}^{n_1l_1m_1n_2l_2m_2}|n_il_im_iN_iL_iM_i\rangle$, where the quantum numbers $n_il_im_i$ pertain to relative motion of the two particles while $N_iL_iM_i$ to the center-of-mass motion [$m_1+m_2=m_i+M_i$, $(2n_1+l_1)+(2n_2+l_2)=(2n_i+l_i)+(2N_i+L_i)$], since the two-body K matrix is diagonal in the center-of-mass quantum numbers. Further use has been made of the property that the K matrix is diagonal in the total angular momentum $j_i(\mathbf{j}_i=\mathbf{l}_i+\mathbf{S})$ and the spin $S(\mathbf{S}=\mathbf{s}_1+\mathbf{s}_2)$ of the two-nucleon system. Thus the calculation of the K matrix for the extra neutron in the states $J=\frac{5}{2}$ and $J=\frac{3}{2}$ has been carried out. It is explicitly demonstrated that the K matrix is independent of $M(=J_z)$. The actual evaluation of the K matrix is done by expanding in terms of the two-nucleon potential [Eq. (53)]. Since all realistic two-nucleon potentials include a repulsive hard core, this expansion is carried out in terms of the matrix elements of the finite part of the two-nucleon potential evaluated for modified oscillator wave functions which include the effect of the hard core. The numerical calculations are done for the Gammel-Thaler[4] potential to first order so that the only contribution to the nuclear spin-orbit interaction is from the two-nucleon spin-orbit part of the potential. The tensor part of the potential will contribute in the second order, as also the effect of the Pauli exclusion principle and the excitations of the core. The first-order calculation gives a value of −5.95 MeV for the spin-orbit doublet separation in O^{17} as compared to the experimental value[11] of −5.083 MeV. The agreement is expected to improve since the tensor force is noted to contribute a small amount but of the wrong sign to the spin-orbit interaction in nuclei. These higher-order calculations, within the framework of this paper, are quite laborious and we expect to report them subsequently.

APPENDIX A. TABLES OF TALMI COEFFICIENTS

In the Tables VII–XVIII the center-of-mass state $|NLM)$ is written next to the Talmi coefficients.[6] The relative states are given as column headings.

APPENDIX B. RESTRICTION ON THE FORM OF THE K MATRIX ELEMENTS IMPOSED BY CONSERVATION OF ANGULAR MOMENTUM

Since the two-body K matrix conserves the (two-body) total angular momentum J we know that the

TABLE VII. Talmi coefficients for the symmetric core-core states.

$\mathcal{S}\|n_1l_1m_1n_cl_cm_c)$ \ $\|nlm\rangle$	$\|000\rangle$	$\|022\rangle$	$\|021\rangle$	$\|020\rangle$	$\|02\ -1\rangle$	$\|02\ -2\rangle$	$\|100\rangle$
$\mathcal{S}\|000;000)$	$\|000)$						
$\mathcal{S}\|011;000)$	$\|011)$						
$\mathcal{S}\|010;000)$	$\|010)$						
$\mathcal{S}\|01\ -1;000)$	$\|01\ -1)$						
$\mathcal{S}\|011;011)$	$(1/\sqrt{2})\|022)$	$-(1/\sqrt{2})\|000)$					
$\mathcal{S}\|011;010)$	$(1/\sqrt{2})\|021)$		$-(1/\sqrt{2})\|000)$				
$\mathcal{S}\|011;01\ -1)$	$(1/\sqrt{6})\|020)+(1/\sqrt{3})\|100)$			$-(1/\sqrt{6})\|000)$			$-(1/\sqrt{3})\|000)$
$\mathcal{S}\|010;010)$	$(1/\sqrt{3})\|020)-(1/\sqrt{6})\|100)$			$-(1/\sqrt{3})\|000)$			$(1/\sqrt{6})\|000)$
$\mathcal{S}\|010;01\ -1)$	$(1/\sqrt{2})\|02\ -1)$				$-(1/\sqrt{2})\|000)$		
$\mathcal{S}\|01\ -1;01\ -1)$	$(1/\sqrt{2})\|02\ -2)$					$-(1/\sqrt{2})\|000)$	

[11] M. A. Preston, *Physics of the Nucleus* (Addison-Wesley Publishing Co., Inc., Reading, Mass., 1962), p. 184.

TABLE VIII. Talmi coefficients for antisymmetric core states.

$\mathfrak{A}\|n_1l_1m_1n_cl_cm_c)$ \ $\|nlm\rangle$	$\|011\rangle$	$\|010\rangle$	$\|01\ -1\rangle$
$\mathfrak{A}\|011;000)$	$\|000)$		
$\mathfrak{A}\|010;000)$	$\|000)$		
$\mathfrak{A}\|01\ -1;000)$	$\|000)$		
$\mathfrak{A}\|011;010)$	$(1/\sqrt{2})\|010)$	$-(1/\sqrt{2})\|011)$	
$\mathfrak{A}\|011;01\ -1)$	$(1/\sqrt{2})\|01\ -1)$		$-(1/\sqrt{2})\|011)$
$\mathfrak{A}\|010;01\ -1)$		$-(1/\sqrt{2})\|01\ -1)$	$(1/\sqrt{2})\|010)$

matrix elements are of the form

$$\langle nlSJM|K|n'l'S'J'M'\rangle=\delta_{JJ'}\delta_{SS'}k^S{}_{nn'll',J}\,, \quad \text{(B1)}$$

where we have also taken into account that the K matrix derived from the two-body nuclear-force law is diagonal in S. From Eqs. (42), (40a), and (40b) we see that the interaction between the extra neutron of O^{17} with the core can be written as a linear combination of the following three forms:

$$\langle n'l'm|K^1|nlm\rangle\equiv\langle n'l'm|\{2K_{1T}{}^{11}+K_{1T}{}^{00}\}|nlm\rangle \quad \text{(B2a)}$$

$$\langle n'l'm|K^0|nlm\rangle\equiv\langle n'l'm|K_{1T}{}^{00}|nlm\rangle \quad \text{(B2b)}$$

$$\langle n'l'm-1|K^f|nlm\rangle \equiv\langle n'l'm-1|\{K_{1T}{}^{10}+K_{1T}{}^{0\,-1}\}|nlm\rangle, \quad \text{(B2c)}$$

where $T=(1,0)$ for $l=$ (odd, even) for K^1 and K^f and the opposite for K^0. The notation above is, explicitly

$$K_{ST}{}^{M_SM'_S}\equiv\langle SM_S|K_T|SM'_S\rangle. \quad \text{(B3)}$$

In view of Eq. (B1), we write the states $|nlmSM_S\rangle$ in terms of the states $|nlSJM_J\rangle$ using Clebsch-Gordan coefficients:

$$|nlmSM_S\rangle=\sum_J\,(lSmM_S|JM_J)|nlSJM_J\rangle, \quad \text{(B4)}$$

so that the matrix elements become [using Eqs. (B1), (B3), and (B4)],

$$\langle n'l'm'|K_{ST}{}^{M_S'M_S}|nlm\rangle=\sum_J\,(lSmM_S|JM_J)^* \times(l'Sm'M'_S|JM_J)k_{n'nl'l,J}{}^S. \quad \text{(B5)}$$

1. Expansion of $\langle n'l'm|K^1|nlm\rangle$ for $n'l'=nl$

$$\langle nlm|K^1|nlm\rangle=2\langle nlm111|K_T|nlm11\rangle +\langle nlm10|K_T|nlm10\rangle=2\sum_J\,(l1m1|JM)^2k_{nl,J}{}^1 +\sum_J\,(l1m0|JM)^2k_{nl,J}{}^1=\sum_J\,\{A_{lJ}m+B_{lJ}\}k_{nl,J}{}^1, \quad \text{(B6)}$$

where

$$A_{lJ}m+B_{lJ}\equiv\{2(l1m1|JM)^2+(l1m0|JM)^2\}. \quad \text{(B7a)}$$

For the three values of J, the results are

(a) $J=l+1$

$$\{\cdots\}=2\frac{(l+m+2)(l+m+1)}{2(l+1)(2l+1)}+\frac{(l+m+1)(l-m+1)}{(l+1)(2l+1)} =\frac{2l+3}{(l+1)(2l+1)}m+\frac{2l+3}{2l+1}, \quad \text{(B7b)}$$

(b) $J=l$

$$\{\cdots\}=2\frac{(l-m)(l+m+1)}{2l(l+1)} +\frac{m^2}{l(l+1)}=1-\frac{1}{l(l+1)}m, \quad \text{(B7c)}$$

TABLE IX. Talmi coefficients for the symmetric state $\mathcal{S}|022;\,n_cl_cm_c)$.

$\mathcal{S}\|n_1l_1m_1n_cl_cm_c)$	$\|000\rangle$	$\|022\rangle$	$\|021\rangle$	$\|020\rangle$	$\|02\ -1\rangle$	$\|02\ -2\rangle$	$\|100\rangle$
$\mathcal{S}\|022;000)$	$(1/\sqrt{2})\|022\rangle$	$(1/\sqrt{2})\|000)$					
$\mathcal{S}\|022;011)$	$\sqrt{\tfrac{3}{4}}\|033)$	$-\tfrac{1}{2}\|011)$					
$\mathcal{S}\|022;010)$	$\tfrac{1}{2}\|032)$	$\tfrac{1}{2}\|010)$	$-(1/\sqrt{2})\|011)$				
$\mathcal{S}\|022;01\ -1)$	$(1/\sqrt{20})\|031)+(1/\sqrt{5})\|111)$	$\tfrac{1}{2}\|11\ -1)$	0	$-(1/\sqrt{6})\|011)$			$-(1/\sqrt{3})\|011)$
$\sum$ squares	7/4	5/4	$\tfrac{1}{2}$	$\tfrac{1}{6}$	0	0	$\tfrac{1}{3}$

TABLE X. Talmi coefficients for the symmetric states $\mathcal{S}|021;\,n_cl_cm_c)$.

$\mathcal{S}\|n_1l_1m_1n_cl_cm_c)$	$\|000\rangle$	$\|022\rangle$	$\|021\rangle$	$\|020\rangle$	$\|02\ -1\rangle$	$\|02\ -2\rangle$	$\|100\rangle$
$\mathcal{S}\|021;000)$	$(1/\sqrt{2})\|021)$		$(1/\sqrt{2})\|000)$				
$\mathcal{S}\|021;011)$	$(1/\sqrt{2})\|032)$	$-(1/\sqrt{2})\|010)$					
$\mathcal{S}\|021;010)$	$\sqrt{\tfrac{2}{5}}\|031)-(1/\sqrt{10})\|111)$			$-(1/\sqrt{3})\|011)$			$(1/\sqrt{6})\|011)$
$\mathcal{S}\|021;01\ -1)$	$\sqrt{(3/20)}\|030)+(1/\sqrt{10})\|110)$		$\tfrac{1}{2}\|01\ -1)$	$-(1/\sqrt{12})\|010)$	$-\tfrac{1}{2}\|011)$		$-(1/\sqrt{6})\|010)$
$\sum$ squares	7/4	$\tfrac{1}{2}$	$\tfrac{3}{4}$	5/12	$\tfrac{1}{4}$	0	$\tfrac{1}{3}$

(c) $J=l-1$

$$\{\cdots\}=2\frac{(l-m)(l-m-1)}{2l(2l+1)}+\frac{(l-m)(l+m)}{l(2l+1)}$$

$$=\frac{2l-1}{2l+1}-\frac{2l-1}{l(2l+1)}m. \quad \text{(B7d)}$$

2. Expansion of $\langle n'l'm-1|K^f|nlm\rangle$ for the Case $n'l'=nl$

$$\langle n'l'm-1|K_T{}^f|nlm\rangle=\langle nlm-111|K_T|nlm10\rangle$$
$$+\langle nlm-1\,10|K_T|nlm1\,-1\rangle$$
$$=\sum_J (l1\,m-1\,1|Jm)(l1m0|JM)k_{nl,J}{}^1$$
$$+\sum_J (l1\,m-1\,0|Jm-1)(l1m-1|Jm-1)k_{nl,J}{}^1$$
$$=\sum_J \{\cdots\}k_{nl,J}{}^1. \quad \text{(B8)}$$

The curly brackets on the right hand side of Eq. (B8) are evaluated below:

(a) for $J=l+1$

$$\{\cdots\}=\left[\frac{(l+m+1)(l+m)}{2(l+1)(2l+1)}\right]^{1/2}\left[\frac{(l+1)^2-m^2}{(l+1)(2l+1)}\right]^{1/2}$$
$$+\left[\frac{(l+1)^2-(m-1)^2}{(l+1)(2l+1)}\right]^{1/2}\left[\frac{(l-m+2)(l-m+1)}{2(l+1)(2l+1)}\right]^{1/2}$$
$$=\left[\frac{(l+m)(l-m+1)}{2}\right]^{1/2}\left[\frac{2l+3}{(l+1)(2l+1)}\right], \quad \text{(B9a)}$$

(b) for $J=l$

$$\{\cdots\}=-\left[\frac{(l+m)(l-m+1)}{2l(l+1)}\right]^{1/2}\left[\frac{m^2}{l(l+1)}\right]^{1/2}$$
$$+\left[\frac{(m-1)^2}{l(l+1)}\right]^{1/2}\left[\frac{(l-m+1)(l+m)}{2l(l+1)}\right]^{1/2}$$
$$=\left[\frac{(l+m)(l-m+1)}{2}\right]^{1/2}\left[-\frac{1}{l(l+1)}\right], \quad \text{(B9b)}$$

(c) for $J=l-1$

$$\{\cdots\}=-\left[\frac{(l+m)(l-m)^2(l-m+1)}{2l^2(2l+1)^2}\right]^{1/2}$$
$$-\left[\frac{(l+m-1)^2(l+m)(l-m+1)}{2l^2(2l+1)^2}\right]$$
$$=\left[\frac{(l+m)(l-m+1)}{2}\right]^{1/2}\left[-\frac{2l-1}{l(2l+1)}\right]. \quad \text{(B9c)}$$

TABLE XI. Talmi coefficients for the symmetric states $\mathcal{S}|020;n_cl_cm_c\rangle$.

$\mathcal{S}\|n_1l_1m_1n_cl_cm_c\rangle$	$\|000\rangle$	$\|022\rangle$	$\|021\rangle$	$\|020\rangle$	$\|02\,-1\rangle$	$\|02\,-2\rangle$	$\|100\rangle$
$\mathcal{S}\|020;000)$	$(1/\sqrt{2})\|020)$			$(1/\sqrt{2})\|000)$			
$\mathcal{S}\|020;011)$	$\sqrt{\tfrac{3}{10}}\|031)+(1/\sqrt{30})\|111)$	$-(1/\sqrt{6})\|01\,-1)$	$-(1/\sqrt{3})\|010)$	$\tfrac{1}{3}\|011)$			$-(1/\sqrt{18})\|011)$
$\mathcal{S}\|020;010)$	$\sqrt{(9/20)}\|030)-\sqrt{(2/15)}\|110)$		$-(1/\sqrt{12})\|11\,-1)$	$-\tfrac{1}{6}\|010)$	$-(1/\sqrt{12})\|011)$		$\sqrt{(2/9)}\|010)$
$\mathcal{S}\|020;01\,-1)$	$\sqrt{\tfrac{3}{10}}\|03\,-1)+(1/\sqrt{30})\|11\,-1)$			$\tfrac{1}{3}\|01\,-1)$	$-(1/\sqrt{3})\|010)$	$-(1/\sqrt{6})\|011)$	$(1/\sqrt{13})\|01\,-1)$
$\sum$ squares	7/4	$\tfrac{1}{6}$	5/12	$\tfrac{3}{4}$	5/12	$\tfrac{1}{6}$	$\tfrac{1}{3}$

TABLE XII. Talmi coefficients for the antisymmetric states $\mathcal{A}|022;n_cl_cm_c\rangle$.

$\mathcal{A}\|n_1l_1m_1n_cl_cm_c\rangle$	$\|011\rangle$	$\|010\rangle$	$\|01\,-1\rangle$	$\|033\rangle$	$\|032\rangle$	$\|031\rangle$	$\|111\rangle$
$\mathcal{A}\|022;000)$	$\|011)$						
$\mathcal{A}\|022;011)$	$-\tfrac{1}{2}\|022)$			$\sqrt{\tfrac{3}{4}}\|000)$			
$\mathcal{A}\|022;010)$	$-(1/\sqrt{2})\|021)$	$\tfrac{1}{2}\|022)$			$\tfrac{1}{2}\|000)$		
$\mathcal{A}\|022;01\,-1)$	$-(1/\sqrt{6})\|020)-(1/\sqrt{3})\|100)$		$\tfrac{1}{2}\|022)$			$(1/\sqrt{20})\|000)$	$(1/\sqrt{5})\|000)$
$\sum$ squares	9/4	$\tfrac{1}{4}$	$\tfrac{1}{4}$	$\tfrac{3}{4}$	$\tfrac{1}{4}$	1/20	$\tfrac{1}{5}$

TABLE XIII. Talmi coefficients for the antisymmetric states $\mathcal{A}|021; n_cl_cm_c)$

$\mathcal{A}\|n_1l_1m_1n_cl_cm_c)$	$\|011\rangle$	$\|010\rangle$	$\|01\ -1\rangle$	$\|032\rangle$	$\|031\rangle$	$\|030\rangle$	$\|111\rangle$	$\|110\rangle$
$\mathcal{A}\|021;000)$	$(1/\sqrt{2})\|010)$	$(1/\sqrt{2})\|011)$						
$\mathcal{A}\|021;011)$		$-(1/\sqrt{2})\|022)$		$(1/\sqrt{2})\|000)$				
$\mathcal{A}\|021;010)$	$-(1/\sqrt{3})\|020)+(1/\sqrt{6})\|100)$				$\sqrt{\frac{2}{5}}\|000)$		$-(1/\sqrt{10})\|000)$	
$\mathcal{A}\|021;01\ -1)$	$-\frac{1}{2}\|02\ -1)$	$-(1/\sqrt{12})\|020)-(1/\sqrt{6})\|100)$	$\frac{1}{2}\|021)$			$\sqrt{(3/20)}\|000)$		$(1/\sqrt{10})\|000)$
$\sum$ squares	5/4	5/4	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{2}{5}$	3/20	$\frac{1}{10}$	$\frac{1}{10}$

TABLE XIV. Talmi coefficients for the antisymmetric state $\mathcal{A}|020; n_cl_cm_c)$.

$\mathcal{A}\|n_1l_1m_1n_cl_cm_c)$	$\|011\rangle$	$\|010\rangle$	$\|01\ -1\rangle$	$\|031\rangle$	$\|030\rangle$	$\|03\ -1\rangle$	$\|111\rangle$	$\|110\rangle$	$\|11\ -1\rangle$
$\mathcal{A}\|020;000)$	$(1/\sqrt{6})\|01\ -1)$	$\sqrt{\frac{2}{3}}\|010)$	$(1/\sqrt{6})\|011)$						
$\mathcal{A}\|020;011)$	$\frac{1}{3}\|020)-(1/\sqrt{18})\|100)$	$-(1/\sqrt{3})\|021)$	$-(1/\sqrt{6})\|022)$	$\sqrt{\frac{3}{10}}\|000)$			$(1/\sqrt{30})\|000)$		
$\mathcal{A}\|020;010)$	$-(1/\sqrt{12})\|02\ -1)$	$-\frac{1}{6}\|020)+\sqrt{(2/9)}\|100)$	$-(1/\sqrt{12})\|021)$		$\sqrt{(9/20)}\|000)$			$-\sqrt{(2/15)}\|000)$	
$\mathcal{A}\|020;01\ -1)$	$-(1/\sqrt{6})\|02\ -2)$	$-(1/\sqrt{3})\|021)$	$\frac{1}{3}\|020)-(1/\sqrt{18})\|100)$			$\sqrt{\frac{3}{10}}\|000)$			$(1/\sqrt{30})\|000)$
$\sum$ squares	7/12	19/12	7/12	$\frac{3}{10}$	9/20	$\frac{3}{10}$	1/30	2/15	1/30

We see that

$$\langle nlm-1|K^f|nlm\rangle=\left[\frac{(l+m)(l-m+1)}{2}\right]^{1/2}\times\sum_J A_{lJ}k_{nl,J}^1, \quad \text{(B10)}$$

where the A_{lJ} are the same as those for $\langle nlm|K_T^1|nlm\rangle$.

3. Expansion of $\langle n'l'm|K^1|nlm\rangle$ for the Case $l'=l\pm2$; $n'=n\mp1$

Here, we must have $J=l\pm1$:

$$\begin{aligned}\langle n'l'm|\{2K_{1T}^{11}+K_{1T}^{00}\}|nlm\rangle&=\{2(l'1m1|l\pm1\ m+1)(lSm1|l\pm1\ m\pm1)\\&\quad+(l'1m0|l\pm1\ m)(l1m0|l\pm1\ m)\}\\&\quad\times\langle n'l'1\ l\pm1\ M|K_T|nl1\ l\pm1\ M\rangle.\quad \text{(B11)}\end{aligned}$$

TABLE XV. Spin-flip coefficients for n, l, $m'=022$ (symmetric).

	$\langle 022\|K_s^f\|021\rangle$	$\langle 021\|K_s^f\|020\rangle$	$\langle 020\|K_s^f\|02\ -1\rangle$	$\langle 02-1\|K_s^f\|02\ -2\rangle$
$(022;000\|\mathcal{S}^\dagger K_s\mathcal{S}\|021;000)$	$\left(\frac{1}{\sqrt2}\right)\left(\frac{1}{\sqrt2}\right)$	0	0	0
$(022;011\|\mathcal{S}^\dagger K_s\mathcal{S}\|021;011)$	0	0	0	0
$(022;010\|\mathcal{S}^\dagger K_s\mathcal{S}\|021;010)$	0	$\left(-\frac{1}{\sqrt2}\right)\left(-\frac{1}{\sqrt3}\right)$	0	0
$(022;01\ -1\|\mathcal{S}K_s\mathcal{S}\|021;01\ -1)$	$\left(\frac{1}{2}\right)\left(\frac{1}{2}\right)$	0	$\left(-\frac{1}{\sqrt6}\right)\left(-\frac{1}{2}\right)$	0
Sum	$\frac{3}{4}(K_s^f)_{022}$	$(1/\sqrt6)(K_s^f)_{021}$	$(1/2\sqrt6)(K_s^f)_{021}$	

TABLE XVI. Spin-flip coefficients for n, l, $m'=022$ (antisymmetric).

	$\langle 011\|K_a^f\|010\rangle$	$\langle 010\|K_a^f\|01\ -1)$	$(K_a^f)_{033}$	$(K_a^f)_{032}$	$(K_a^f)_{031}$	$(K_a^f)_{111}$
$(022;000\|\mathcal{A}^\dagger K_a^f\mathcal{A}\|021;000)$	$(1)\left(\frac{1}{\sqrt2}\right)$					
$(022;011\|\mathcal{A}^\dagger K_a^f\mathcal{A}\|021;011)$	$\left(-\frac{1}{\sqrt2}\right)\left(-\frac{1}{2}\right)$		$\left(\frac{3}{4}\right)^{1/2}\left(\frac{1}{2}\right)^{1/2}$			
$(022;010\|\mathcal{A}^\dagger K_a^f\mathcal{A}\|021;010)$	0			$\frac{1}{2}\left(\frac{2}{5}\right)^{1/2}$		
$(022;01\ -1\|\mathcal{A}^\dagger K_a^f\mathcal{A}\|021;01\ -1)$	$\left(-\frac{1}{\sqrt6}\right)\left(-\frac{1}{\sqrt{12}}\right)$	$\left(-\frac{1}{\sqrt3}\right)\left(-\frac{1}{\sqrt6}\right)$			$\frac{1}{\sqrt{20}}\left(\frac{3}{20}\right)^{1/2}$	$\frac{1}{\sqrt5}\frac{1}{\sqrt{10}}$
Sum	$(2/\sqrt2)(K_a^f)_{011}$					

TABLE XVII. Spin-flip coefficients for n, l, $m'=021$ (symmetric).

	$(K_s^f)_{022}$	$(K_s^f)_{021}$	$(K_s^f)_{020}$	$(K_s^f)_{02-1}$
$(021;000\|\mathcal{S}^\dagger K_s\mathcal{S}\|020;000)$	$1/\sqrt6$	$\frac{1}{2}$		
$(021;011\|\mathcal{S}^\dagger K_s\mathcal{S}\|020;011)$				
$(021;010\|\mathcal{S}^\dagger K_s\mathcal{S}\|020;010)$			$1/\sqrt{36}$	
$(021;01\ -1\|\mathcal{S}^\dagger K_s\mathcal{S}\|020;01\ -1)$		$\frac{1}{6}$	$1/\sqrt{36}$	$1/2\sqrt6$
Sum	$(1/\sqrt6)(K_s^f)_{022}$	$\frac{2}{3}(K_s^f)_{021}$	$\frac{1}{3}(K_s^f)_{021}$	$(1/2\sqrt6)(K_s^f)_{022}$

TABLE XVIII. Spin-flip coefficients for n, l, $m'=021$ (antisymmetric).

	$(K_a{}^f)_{011}$	$(K_a{}^f)_{010}$	$(K_a{}^f)_{032}$	$(K_a{}^f)_{031}$	$(K_a{}^f)_{030}$	$(K_a{}^f)_{111}$	$(K_a{}^f)_{110}$
$(021;000\|\mathfrak{a}^\dagger K_a\mathfrak{a}\|020;000)$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{12}}$					
$(021;011\|\mathfrak{a}^\dagger K_a\mathfrak{a}\|020;011)$		$\frac{1}{\sqrt{12}}$	$\left(\frac{3}{20}\right)^{1/2}$				
$(021;010\|\mathfrak{a}^\dagger K_a\mathfrak{a}\|020;010)$	$\frac{1}{6\sqrt{3}}+\frac{1}{3\sqrt{3}}$			$\left(\frac{9}{50}\right)^{1/2}$		$\left(\frac{2[illegible]}{150}\right)^{1/2}$	
$(021;01\,-1\|\mathfrak{a}^\dagger K_a\mathfrak{a}\|020;01\,-1)$	$\frac{1}{2\sqrt{3}}$	$\frac{-1}{3\sqrt{12}}+\frac{1}{6\sqrt{3}}$			$\frac{3}{10\sqrt{2}}$		$\frac{1}{10\sqrt{3}}$
Sum	$\frac{3}{\sqrt{3}}(K_a{}^f)_{011}$		$\frac{3}{2\sqrt{15}}(K_a{}^f)_{032}$	$\frac{9}{10\sqrt{2}}(K_a{}^f)_{031}$		$\frac{3}{10\sqrt{3}}(K_a{}^f)_{111}$	

The coefficient in brackets is zero, for all l, m, as can be verified by direct substitution.

4. Expansion of $\langle n'l'm-1|K^f|nlm\rangle$ for the Case $l'=l\pm 2$; $n'=n\mp 1$

In this case also, we must have $J=l\pm 1$:

$$\langle n'l'm-1|\{K_{1T}{}^{10}+K_{1T}{}^{0\,-1}\}|nlm\rangle$$
$$=\{(l\pm 2\;1\;m-1\;1|l\pm 1\;m)(l1m0|l\pm 1\;m)$$
$$+(l\pm 2\;1\;m-1\;0|l\pm 1\;m-1)(l1m\;-1|l\pm 1\;m-1)\}$$
$$\times\langle n'l'1\;l\pm 1\;M|K_T|nl1\;l\pm 1\;M\rangle. \quad \text{(B12)}$$

The coefficient in brackets is zero, for any l,m, as can be seen by direct substitution.

5. General Form

From the above, we see that we can write the $\langle n'l'm'|\times K|nlm\rangle$ in terms of the $k_{nl,J}{}^S$ as follows:

$$\langle n'l'm|K_T{}^0|nlm\rangle\equiv K_{nlm}{}^0=k_{nl,l}{}^0 \quad \text{(B13a)}$$

$$\langle nlm|K_T{}^1|nlm\rangle\equiv K_{nlm}{}^1=\sum_{J=l-1}^{l+1}(A_{lJ}m+B_{lJ})k_{nl,J}{}^1 \quad \text{(B13b)}$$

$$\langle nlm-1|K_T{}^f|nlm\rangle\equiv K_{nlm}{}^f=\left[\frac{(l+m)(l-m+1)}{2}\right]^{1/2}\sum_{J=l-1}^{+}A_{lJ}k_{nl,J}{}^1 \quad \text{(B13c)}$$

$$\langle n\mp 1\;l\pm 2\;m|K_T{}^S|nlm\rangle=0=\langle n\mp 1\;l\pm 2\;m-1|K_T{}^f|nlm\rangle, \quad \text{(B14)}$$

where A_{lJ} and B_{lJ} are given in Table XIX.

TABLE XIX. Values of A_{lJ} and B_{lJ} in Eqs. (B13a)–(B13c).

$J=$	$l+1$	l	$l-1$
$A_{lJ}=$	$\frac{2l+3}{(l+1)(2l+1)}$	$-\frac{1}{l(l+1)}$	$-\frac{2l-1}{l(2l-1)}$
$B_{lJ}=$	$\frac{2l+3}{2l+1}$	1	$\frac{2l-1}{2l+1}$