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Unitary-Model-Operator Approach to Nuclear-Structure Physics. II. Applications*

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Results are reported for Hartree-Fock calculations carried out with an effective interaction derived from the Yale potential. The spherical nuclei O^{16} and Ca^{40} are considered. The orbitals are expanded in terms of harmonic-oscillator functions, and the dependence of the results on the number of oscillator functions used and upon the oscillator size parameter is studied. The importance of various second-order terms is considered using a simple approximation for the Pauli operator and the energy denominators. For the second-order terms in the tensor interaction, some spectral corrections to the simplified energy denominators are made. Reasonable results are obtained for the nuclei considered; however, the spectral corrections to the simplified energy denominators are found to provide an important correction to the calculated binding energy. It is concluded that an improved treatment of the energy denominators is required to improve the accuracy of the results reported here. Tables of the effective interaction used in these calculations are presented in an Appendix.

I. INTRODUCTION

ONE of the fundamental problems in the study of nuclear structure is to obtain a satisfactory understanding of the static properties of nuclei such as binding energies, moments, spectra, etc. These properties depend upon the nature of the force acting between nucleons inside the nucleus. It is not unreasonable to assume that the potentials that describe the scattering of free nucleons[1,2] may be used in the study of the properties of finite nuclei or nuclear matter. These potentials exhibit strong repulsion at short distances and this fact greatly complicates nuclear-structure calculations. Brueckner[3] and others[4] have developed theories based upon two-particle correlations (reaction matrix theories) and some applications have been made to the study of the properties of finite nuclei.[3]

In a preceding work,[5] referred to as I in the following, a method has been developed which allows one to derive an effective Hamiltonian starting from a Hamiltonian involving strongly repulsive forces.[5-7] The effective Hamiltonian is generated using a model-operator approach; however, the calculational procedures and results do not differ significantly from the reaction matrix approach to the effective interaction problem based on the Moszkowski-Scott[4] separation method. The novel features of the methods used here include the introduction of pseudopotentials to achieve healing of the correlated wave functions in those states where the interaction is essentially repulsive. Also the use of a harmonic-oscillator basis involving oscillator functions of several nodes allows one to improve the orbitals used in the direction of eliminating the one-particle one-hole corrections to the binding energy. Indeed, the main concern of this work is the application of the Hartree-Fock method to the effective Hamiltonian. It is well known that the concepts of the Hartree-Fock theory underlie most nuclear models which are used in nuclear-structure physics, and a calculational procedure which generates the nuclear Hartree-Fock field, binding energies, deformations, spin-orbit splittings, etc., is highly desirable.

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[1] K. E. Lassila, M. H. Hull, Jr., H. M. Ruppel, F. A. McDonald, and G. Breit, Phys. Rev. **126**, 881 (1962).

[2] T. Hamada and I. D. Johnston, Nucl. Phys. **34**, 382 (1962); T. Hamada, V. Nakamura, and R. Tomagaki, Progr. Theoret. Phys. (Kyoto) **33**, 769(L) (1965).

[3] K. A. Brueckner, J. L. Gammel, and H. Weitzner, Phys. Rev. **110**, 431 (1958); K. A. Brueckner, A. M. Lockett, and M. Rotenberg, *ibid.* **121**, 255 (1961); K. S. Masterson, Jr., and A. M. Lockett, *ibid.* **127**, 776 (1963); H. S. Kohler and R. J. McCarthy (unpublished); A. D. MacKellar and R. L. Becker, Phys. Letters **18**, 308 (1965).

[4] L. C. Gomes, J. D. Walecka, and V. F. Weisskopf, Ann. Phys. (N. Y.) **3**, 241 (1958), H. A. Bethe and J. Goldstone, Proc. Roy. Soc. (London) **A238**, 551 (1957); H. A. Bethe, B. H. Brandow, and A. G. Petschek, Phys. Rev. **129**, 225 (1963); S. A. Moszkowski and B. L. Scott, Ann. Phys. (N. Y.) **11**, 65 (1960); H. A. Bethe, Phys. Rev. **138**, B804 (1965).

[5] C. M. Shakin, Y. R. Waghmare, and M. H. Hull, Jr., preceding paper, Phys. Rev. **161**, 1006 (1967).

[6] C. M. Shakin and Y. R. Waghmare, Phys. Rev. Letters **16**, 403 (1966).

[7] M. H. Hull, Jr., and C. M. Shakin, Phys. Letters **19**, 506 (1965).

Clearly, the application of the Hartree-Fock method to an *effective* Hamiltonian does not provide one with an upper bound for the binding energy. The justification of the use of the Hartree-Fock method must be found in the fact that it provides wave functions which are related in a self-consistent manner to the effective interaction. Once this self-consistency is achieved there are no first-order corrections of the one-particle one-hole type to the ground state. (The treatment of the second-order terms due to the tensor force given in I also takes into account some very important two-particle, two-hole excitations involving high-energy orbitals. These tensor force effects will greatly complicate any attempt to apply Hartree-Fock theory in its usual form, even with nonsingular forces, since the tensor correlations are responsible for a large part of the binding energy of the nucleus.)

One essential difficulty remains in that the effective interaction generated depends somewhat on the dispersive character of the medium. In the formalism of I, the use of harmonic-oscillator wave functions as a basis is particularly simple if the dispersive effects of the medium are represented by harmonic-oscillator potentials. This choice allows for a simple separation of the center-of-mass and relative motion of an interacting pair. It is fairly difficult to give an accurate estimate of the correction due to the use of this approximation and for the results reported here this limitation should be kept in mind.

II. THEORY

In this section a brief resumé of the effective interaction method is presented, the details of which are given in I. Given a Hamiltonian H, an effective interaction $\tilde{H}$ is determined by using a unitary operator e^{iS} such that

$$\begin{aligned}\tilde{H}=e^{-iS}He^{iS}=\sum t_{n_1n_2}a_{n_1}{}^\dagger a_{n_2}\\ +\tfrac{1}{2}\sum a_{n_1}{}^\dagger a_{n_2}{}^\dagger\langle n_1n_2|e^{-iS}(t_1+t_2+U_1+U_2+v_{12})e^{iS}\\ -(t_1+t_2+U_1+U_2)|n_3n_4\rangle a_{n_4}a_{n_3}+\cdots,\end{aligned}\quad(1)$$

where t is the kinetic energy operator, and v_{12} is the nucleon-nucleon potential exhibiting strong repulsion at short distances. The single-particle potentials U_1 and U_2, which represent the dispersive properties of the medium and arise from the analysis of the three-body terms in the cluster expansion of $\tilde{H}$ are approximated by harmonic-oscillator forms, namely, $U_1=\frac{1}{2}kr_1{}^2$, $U_2=\frac{1}{2}kr_2{}^2$. The potential v_{12} is divided into a short-range part $v_{12}{}^S$ and a long-range part $v_{12}{}^l$, so as to satisfy the following equations[5]:

$$\begin{aligned}(t_1+t_2+U_1+U_2+v_{12}{}^s)\psi_{n_1n_2}(r_1,r_2)=(\epsilon_{n_1}+\epsilon_{n_2})\psi_{n_1n_2}(r_1,r_2),\\ (t_1+t_2+U_1+U_2)\phi_{n_1n_2}(r_1,r_2)=(\epsilon_{n_1}+\epsilon_{n_2})\phi_{n_1n_2}(r_1,r_2),\end{aligned}\quad(2)$$

where the subscripts n_1 and n_2 refer to the quantities (n,l,j,m) necessary to specify the orbitals for particle motion in harmonic-oscillator potential. The short-range part of the potential, $v_{12}{}^s$, gives no energy shift in the correlated wave function $\psi_{n_1n_2}$ relative to the unperturbed wave functions $\phi_{n_1n_2}$. One finds

$$\begin{aligned}\tilde{H}=\sum t_{n_1n_2}a_{n_1}{}^\dagger a_{n_2}+(\tfrac{1}{2})\sum a_{n_1}{}^\dagger a_{n_2}{}^\dagger\\ \times\langle\psi_{n_1n_2}|v_{12}{}^l|\psi_{n_3n_4}\rangle a_{n_3}a_{n_4}+\cdots,\end{aligned}\quad(3)$$

where we have used

$$e^{iS}\phi_{n_1n_2}=\psi_{n_1n_2}.\quad(4)$$

The distance at which $v_{12}{}^s$ and $v_{12}{}^l$ are separated is called the "healing distance."

In most cases it has been necessary to extend this elementary separation procedure. Generally, a state-dependent pseudopotential VP is added and v_{12} is written as

$$v_{12}=(v_{12}{}^s+VP)+(v_{12}{}^s-VP).\quad(5)$$

This pseudopotential method is used in those states of relative motion where the interaction is repulsive and also in the ${}^1S_0$ and ${}^3S_1$ states. The pseudopotentials are chosen to maintain healing of the correlated wave at about 1 F for the various states of relative motion. For simplicity, the form of the pseudopotential was taken to be constant (attractive) and nonzero from the core of the Yale potential[1] out to about 1 F.

For the ${}^1S_0$ and ${}^3S_1$ states the strength of the pseudopotential varies significantly with the number of modes in the relative wave function. For the ${}^1P_1$, ${}^3P_0$, ${}^3P_1$, ${}^3D_1$, ${}^3D_2$, and ${}^3D_3$ states pseudopotentials are also used but it was sufficient to use a constant value of the pseudopotentials in these states. For these latter states, once the pseudopotential was fixed, the variation of the healing distance with the number of modes was negligible. As discussed in I, the use of a mode- (or energy) dependent pseudopotential makes the effective interaction non-Hermitian. For the purposes of these calculations the matrix elements of the effective interaction in the ${}^1S_0$ and ${}^3S_1$ states off-diagonal in n, the number of modes in the oscillator wave function, was averaged. This procedure is not very satisfactory and a method for overcoming this difficulty was indicated in I but has not been applied as yet. A discussion of the choice of healing distances and pseudopotentials was given in I.

The parts of the tensor force diagonal in l, the relative orbital angular momentum, are included in Eq. (3). The part of the tensor force off-diagonal in l, $v_T{}^{\text{OD}}$, is treated in perturbation theory *in the correlated basis*. To lowest order $\tilde{H}$ becomes

$$\begin{aligned}\tilde{H}=\sum t_{n_1n_2}a_{n_1}{}^\dagger a_{n_3}+\tfrac{1}{2}\sum a_{n_1}{}^\dagger a_{n_2}{}^\dagger\\ \times\langle\psi_{n_1n_2}|v_{12}{}^l+v_T{}^{\text{OD}}|\psi_{n_3n_4}\rangle a_{n_3}a_{n_4}+\cdots.\end{aligned}\quad(6)$$

Now, it is well known that the tensor force contributes significantly in second order, the main feature being the admixture of a short-range ${}^3D_1$ wave to the ${}^3S_1$ state of relative motion. This admixture involves high-energy orbitals. This effect of the tensor force may be included by extending the definition of e^{iS} to include a tensor correlation; i.e., Eq. (4) is modified to read

$$e^{iS}\phi_{n_1n_2}=\psi_{n_1n_2}+(Q/e)v_T^{\mathrm{OD}}\psi_{n_1n_2}\,, \tag{7}$$

where $\psi_{n_1n_2}$ contains only central correlations. Here, e is an appropriate energy denominator and Q is a projection operator. If we make the approximation

$$\epsilon_{n_1}+\epsilon_{n_2}\simeq\epsilon_{n_3}+\epsilon_{n_4}\simeq\Delta\,,$$

and define $e=-(t_1+t_2+U_1+U_2-\Delta)$, we find

$$\tilde{H}=\sum t_{n_1n_2}a_{n_1}{}^{\dagger}a_{n_2}+\tfrac{1}{2}\sum a_{n_1}{}^{\dagger}a_{n_2}{}^{\dagger}a_{n_4}a_{n_3}$$
$$\times\langle\psi_{n_1n_2}|\,(v_{12}{}^{l}-VP)+v_T{}^{\mathrm{OD}}+v_T{}^{\mathrm{OD}}\frac{Q}{e}v_T{}^{\mathrm{OD}}|\psi_{n_3n_4}\rangle\,, \tag{8}$$

where the presence of the pseudopotential term VP has been indicated. The approximation used for the energy denominator in Eq. (7) is reasonable as the orbitals admixed by the tensor force are of quite high energy. The exact specification of the energies of the occupied orbitals is not very important for semiquantitative results; however, to obtain results accurate to 1 or 2 MeV per particle a better treatment of the energy denominators is required. Estimates of the error involved in the simple treatment of the energy denominators are given in the next section.

In a similar fashion second-order effects in VP may be included as VP is of short range and will introduce further short-range correlations when taken to higher order.

Thus,

$$\tilde{H}=\sum t_{n_1n_2}a_{n_1}{}^{\dagger}a_{n_2}+\tfrac{1}{2}\sum a_{n_1}{}^{\dagger}a_{n_2}{}^{\dagger}a_{n_3}a_{n_4}$$
$$\times\langle\psi_{n_1n_2}|\,(v_{12}{}^{l}-VP)+v_T{}^{\mathrm{OD}}+v_T{}^{\mathrm{OD}}(Q/e)v_T{}^{\mathrm{OD}}$$
$$+VP(Q/e)VP|\psi_{n_3n_4}\rangle\,, \tag{9}$$

where we have neglected cross terms in VP and $v_T{}^{\mathrm{OD}}$ which are expected to be small. Calculations have been carried out for the effective interactions of Eqs. (8) and (9) so that the effects of the second-order terms in VP may be determined separately.

In the application of the Hartree-Fock method to the effective interaction the expansion of the orbitals in harmonic-oscillator functions is used.[8] The usual Hartree-Fock equations to be solved are

$$\langle\alpha|t|\beta\rangle+\langle\alpha|U|\beta\rangle=\epsilon_\alpha\delta_{\alpha\beta}\,, \tag{10}$$

where t is the kinetic-energy operator and the single-particle potential U is defined as

$$\langle\alpha|U|\beta\rangle=\sum_{\gamma=1}^{A}\left[\langle\alpha\gamma|v_{\mathrm{eff}}|\beta\gamma\rangle-\langle\alpha\gamma|v_{\mathrm{eff}}|\gamma\beta\rangle\right]. \tag{11}$$

The wave functions are expanded as

$$\psi_\alpha(r)=\sum_n C^\alpha{}_n\phi_n(r)\,, \tag{12}$$

where the ϕ's are the harmonic-oscillator functions. Substitution of Eq. (12) into Eq. (10) yields

$$\sum_{n_1'}\left[\langle n_1|t|n_1'\rangle+\langle n_1|U|n_1'\rangle\right]C_{n_1'}{}^{\alpha}=\epsilon_\alpha C_{n_1}{}^{\alpha}\,, \tag{13}$$

where

$$\langle n_1|U|n_1'\rangle=\sum_{n_2,n_2'}\rho_{n_1n_2'}\left[\langle n_1n_2|v_{\mathrm{eff}}|n_1'n_2'\rangle\right.$$
$$\left.-\langle n_1n_2|v_{\mathrm{eff}}|n_2'n_1'\rangle\right] \tag{14}$$

and

$$\rho_{n_2n_2'}=\sum_{\gamma=1}^{A}C_{n_2}{}^{\gamma}C_{n_2'}{}^{\gamma}.$$

Then, the binding energy is given by

$$E_0=\sum_{n_1n_1'}\rho_{n_1n_1'}\left[\langle n_1|t|n_1'\rangle+\tfrac{1}{2}\langle n_1|U|n_1'\rangle\right].$$

III. RESULTS OF HARTREE-FOCK CALCULATIONS

In this section calculations for the closed-shell nuclei O^{16} and Ca^{40} are reported. These calculations were made using the effective interaction derived from the Yale potential. The matrix elements used are tabulated in the Appendix.

The Hartree-Fock equations were solved by an iteration procedure[8] for various values of $b=(\hbar/M\omega)^{1/2}$, the oscillator size parameter. To test the effects of including various terms of the effective interaction several different calculations were done. First, no second-order terms were included involving VP. Second, the second-order terms in VP were included but only for the relative matrix elements diagonal in n, the number of nodes in the oscillator wave function. Finally, the second-order terms in VP which involve matrix elements off-diagonal in n were included for the P states only. For this latter calculation one should also include the second-order terms in VP off-diagonal in n for the S-states as well; however, these terms were smaller than the uncertainty introduced in the averaging of the S-state interaction matrix elements and it was not considered worthwhile to calculate them.

The results of calculations for O^{16} are presented in Tables I–IV. In Table I are presented the single-particle energies, binding energy per particle, spin-orbit splitting, and root-mean-square radii for a calculation in which three harmonic-oscillator functions were used in the determination of each orbital. The calculation was of the first type mentioned where the second-order terms in VP were neglected. A simple correction was made for the center-of-mass energy and the Coulomb

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[8] J. P. Svenne, thesis, MIT, 1965 (unpublished); R. Muthukrishnan and M. Baranger, Phys. Letters 18, 160 (1965); K. T. R. Davies, S. J. Krieger, and M. Baranger, Nucl. Phys. 84, 545 (1966); A. K. Kerman, J. P. Svenne, and F. M. H. Villars, Phys. Rev. 147, 710 (1966).

TABLE I. Calculated properties of O^{16}. (Second-order terms in VP not included. Three oscillations functions were used for each orbital.)

b (F)	1.50	1.76	2.09	2.17	Experimental
Single-particle energies (MeV)					
$0p_{1/2}$	-43.5	-45.3	-44.9	-41.7	
$0p_{1/2}$	-12.6	-13.1	-13.9	-12.8	-15.65[a] (neutron)
$0p_{3/2}$	-18.1	-18.8	-19.0	-17.4	-21.81 (neutron)
B. E./A (MeV)	-3.01	-3.45	-3.75	-3.30	
E_{Coul}/A (MeV)	0.94	0.94	0.94	0.94	
$E_{\mathrm{c.m.}}/A$ (MeV)	$+0.71$	$+0.71$	$+0.71$	$+0.71$	
B. E./A (MeV) (including Coulomb and c.m. corrections)	-2.78	-3.22	-3.52	-3.17	-7.98
$0p_{3/2}-0p_{1/2}$ splitting (MeV)	5.5	5.7	5.1	4.6	6.2[a]
Rms radius (F)	2.48	2.49	2.53	2.62	2.64[b] (charge rms radius)

[a] B. L. Cohen, Phys. Rev. **130**, 227 (1963).
[b] R. Hofstadter, Ann. Rev. Nucl. Sci. **7**, 231 (1957).

TABLE II. Calculated properties of O^{16}. (Second-order terms in VP included. Three oscillator functions were used for each orbital.)

b (F)	1.50	1.76	2.09	2.17	Experimental
Single-particle energies (MeV)					
$0s_{1/2}$	-55.8	-57.5	-51.9	-48.3	
$0p_{1/2}$	-18.7	-18.9	-17.8	-16.4	-15.65[a] (neutron)
$0p_{3/2}$	-25.4	-25.5	-23.2	-21.3	-21.81 (neutron)
B.E./A (MeV)	-5.97	-5.83	-5.35	-4.76	
E_{Coul}/A (MeV)	0.94	0.94	0.94	0.94	
$E_{\mathrm{c.m.}}/A$ (MeV)	$+0.71$	$+0.71$	$+0.71$	$+0.71$	
B. E./A (MeV) (including Coulomb and c.m. corrections)	-5.74	-5.60	-5.12	-4.53	-7.98
$0p_{3/2}-0p_{1/2}$ splitting (MeV)	6.7	6.6	5.4	4.9	6.2[a]
Rms radius (F)	2.34	2.30	2.43	2.51	2.64[b] (charge rms radius)

[a] B. L. Cohen, Phys. Rev. **130**, 227 (1963).
[b] R. Hofstader, Ann. Rev. Nucl. Sci. **7**, 231 (1957).

energy. These corrections were estimated using the following expressions:

$$E_{\mathrm{Coul}}=\tfrac{3}{5}e^2\frac{Z(Z-1)}{R}, \quad R=1.3A^{1/3},$$

$$E_{\mathrm{c.m.}}=\tfrac{3}{4}\hbar\omega, \quad \hbar\omega=41.6/b^2,$$

where $b=(\hbar/M\omega)^{1/2}$. A rough estimate of the value of b was obtained from comparing the result of the Hartree-Fock calculation for the rms radius with the rms radius obtained assuming pure harmonic-oscillator orbitals. For the O^{16} calculations the center-of-mass correction was estimated with $b\sim 1.66$ F. This correction was held constant in the tables although the calculated rms radius varied somewhat.

Table II contains the results for Hartree-Fock calculations in which the second-order terms in VP were included in the effective-interaction matrix elements. As may be seen from the table, the inclusion of these terms increases the calculated binding energy, the increase being larger for the smaller values of b. There is also a small increase in the calculated spin-orbit splitting and some decrease in the rms radius.

It was of interest to see what results would be obtained if the number of harmonic-oscillator functions used to expand the orbitals was reduced. Table III includes the results for O^{16} when only a single oscillator function was used for each orbit. As might be expected the calculated quantities vary more rapidly as b is changed than in the calculations reported in Tables I and II (for which three oscillator functions were used for each orbital). The greatest difference between the

TABLE III. Calculated properties of O^{16}. (Second-order terms in VP were included and only a single oscillator function was used for each orbital.)

b (F)	1.50	1.76	2.09	2.17
Single-particle energies (MeV)				
$0s_{1/2}$	-57.3	-43.4	-30.2	-27.6
$0p_{1/2}$	-19.0	-16.3	-11.9	-10.6
$0p_{3/2}$	-26.6	-20.0	-13.7	-12.2
B.E./A (MeV) (without Coulomb and c.m. corrections)	-5.82	-4.93	-3.34	-2.63
$0p_{3/2}-0p_{1/2}$ splitting (MeV)	7.6	3.7	1.8	1.6
Rms radius (F)	2.25	2.64	3.14	3.25

Table IV. Single-particle energies and binding energy per particle for O^{16}. The second-order tensor terms were evaluated in a crude self-consistent approximation as discussed in the text. One oscillator function was used for each orbital. Tabulated quantities are given in MeV.

		Iteration			
	$\Delta=20$	(1)	(2)	(3)	(4)
$b=1.50$ F					
$0p_{1/2}$	-19.0	-17.2	-17.4	-17.4	-17.4
$0p_{3/2}$	-26.6	-24.3	-24.7	-24.6	-24.6
$0s_{1/2}$	-57.3	-51.0	-51.9	-51.8	-51.8
B.E./A[a]	-5.82	-4.23	-4.45	-4.42	-4.43
$b=1.76$ F					
$0p_{1/2}$	-16.3	-15.4	-15.5	-15.5	-15.5
$0p_{3/2}$	-20.1	-18.9	-19.0	-19.0	-19.0
$0s_{1/2}$	-43.4	-40.1	-40.5	-40.4	-40.4
B.E./A[a]	-4.93	-4.14	-4.22	-4.21	-4.21
$b=2.09$ F					
$0p_{1/2}$	-11.9	-11.7	-11.7	-11.7	-11.7
$0p_{3/2}$	-13.7	-13.3	-13.4	-13.4	-13.4
$0s_{1/2}$	-30.2	-28.9	-29.0	-29.0	-29.0
B.E./A[a]	-3.34	-3.06	-3.08	-3.08	-3.08
$b=2.17$ F					
$0p_{1/2}$	-10.6	-10.4	-10.4	-10.4	-10.4
$0p_{3/2}$	-12.2	-12.0	-12.0	-12.0	-12.0
$0s_{1/2}$	-27.6	-26.6	-26.7	-26.7	-26.7
B.E./A[a]	-2.88	-2.67	-2.69	-2.69	-2.69

[a] Uncorrected for center-of-mass or Coulomb energy.

results of Table II and III occur for the largest value of b since in this case the single oscillator functions have the poorest overlap with the orbitals determined using a basis of three oscillator functions.

A discussion of the numerical results is in order. For example, in Table II, the quantities calculated are not independent of the basis chosen. Hopefully, if one were to use more oscillator functions in the expansion of the orbitals this dependence on the basis used would be lessened. The value obtained for the spin-orbit splitting is reasonable. The rms radii of Table II are smaller than the experimental value; however, configuration mixing in the ground state would increase this quantity somewhat.[9] As for the binding energies, an important correction arises from the fact that in the evaluation of the $^3S_1$ matrix elements the energy denominator e was taken as

$$-e=(\hbar^2/2m)(k_1^2+k_2^2)+\Delta\,,$$

with $\Delta=20$ MeV. The quantity Δ approximates the binding of the interacting pair in the nucleus. This quantity is actually state-dependent and generally larger than 20 MeV. Correction for this variation can be made using the binding energies of the single-particle orbits as obtained from the Hartree-Fock calculation. This correction is fairly simple to make for the Hartree-Fock calculations involving only a single harmonic-oscillator function for each orbital.

Table XIV exhibits the variation of the diagonal $^3S_1$ matrix elements with the parameter Δ. To study the effect of this variation a Hartree-Fock calculation was carried out for O^{16}. As a simple approximation it was assumed that the relative $^3S_1$ matrix elements depends linearly on Δ with a decrease of 60% in their values on going from $\Delta=20$ MeV to $\Delta=220$ MeV. This approximation corresponds roughly to the behavior of these matrix elements as reported in Table XIV.

The following iterative scheme was adopted. The single-particle energies were obtained by carrying out the Hartree-Fock calculation for O^{16} with the minimum number of orbitals and using the matrix elements calculated with $\Delta=20$. These single-particle energies were then used to obtain an effective Δ for each two-body matrix element. The two-body matrix elements were then recalculated, but in their calculation the $^3S_1$ relative matrix elements were modified to take into account their variation with Δ. For example, if the $0S_{1/2}$ orbit was found to be bound by -50 MeV, say, matrix elements of the form

$$\langle 0S_{1/2}0S_{1/2}JT|v|0S_{1/2}0S_{1/2}JT\rangle$$

were evaluated with the $^3S_1$ *relative* elements modified to correspond to $\Delta=100$ MeV. For matrix elements involving two different orbitals, the Hartree-Fock single-particle energies were again added to obtain an effective Δ. This procedure was iterated until there has no significant change in the single-particle energies and the total binding energy. About four iterations were necessary to achieve this crude form of self-consistency for the energy denominators.

The results obtained using this iteration procedure are presented in Table IV. The first column (for each value of b) gives the single-particle energies and binding energy per particle for $\Delta=20$ MeV. These results are therefore identical to those presented in Table III. The following columns present the results of successive iterations involving modifications of the two-body matrix elements to take into account the dependence of the $^3S_1$ relative elements on the binding energies of the single-particle orbitals. The convergence is quite rapid. The corrections to the binding energy are not very large indicating that a perturbative approach to these spectral corrections should be satisfactory. It is clear from Table IV that the spectral corrections are largest for the smaller values of b since the orbitals were bound most strongly for smaller b. (The approximation, $\Delta=20$ MeV, is clearly poorest for the smaller values of b.)

Table V. Corrections to the O^{16} binding energy (in MeV).

b (F)	Binding energy/A (Table III)	Correction from using more orbitals (Table II)	Spectral correction (Table IV)	Total[a] B.E./A
1.50	-5.82	-0.15	$+1.39$	-4.58
1.76	-4.93	-0.90	$+0.71$	-5.12
2.09	-3.34	-2.01	0.26	-5.09
2.17	-2.63	-2.13	0.19	-4.57

[a] Uncorrected for center-of-mass and Coulomb energy.

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[9] G. E. Brown and G. Jacob, Nucl. Phys. 42, 177 (1963).

TABLE VI. Expansion coefficient for occupied orbitals of O^{16}. The expansion is in terms of oscillator functions having zero, one, and two nodes.

	Calculation of Table I			Calculation of Table II		
	C_0	C_1	C_2	C_0	C_1	C_2
$b=1.5$ F						
$0s_{1/2}$	0.9970	−0.0770	−0.0088	−0.9998	−0.0170	−0.0045
$0p_{3/2}$	0.9887	−0.1460	0.0337	0.9982	−0.0469	0.0335
$0p_{1/2}$	0.9748	−0.1878	0.0683	0.9928	−0.1024	0.0617
$b=1.76$ F						
$0s_{1/2}$	0.9905	0.1361	0.0164	0.9703	0.2342	0.0593
$0p_{3/2}$	−0.9940	−0.0961	−0.0521	0.9739	0.2090	0.0877
$0p_{1/2}$	−0.9969	−0.0320	−0.0710	−0.9844	−0.1492	−0.0928
$b=2.09$ F						
$0s_{1/2}$	0.9470	0.3057	0.0982	0.9267	0.3506	0.1349
$0p_{3/2}$	0.9408	0.3040	0.1495	0.9146	0.3584	0.1867
$0p_{1/2}$	0.9564	0.2510	0.1488	0.9308	0.3166	0.1824
$b=2.17$ F						
$0s_{1/2}$	0.9444	0.3114	0.1053	0.9227	0.3577	0.1435
$0p_{3/2}$	0.9373	0.3087	0.1614	0.9094	0.3649	0.1995
$0p_{1/2}$	0.9519	0.2604	0.1611	0.9246	0.3265	0.1961

It is interesting to compare the results reported in Tables II, III, and IV for the case of the binding energy. This comparison is made in Table V where we have assumed that the corrections to the minimum orbital calculation (Table III) arising from the use of several orbitals (Table II) and the spectral correction of Table IV are additive. It is found that the binding energy is now much less sensitive to the choice of basis functions and also that the binding energy exhibits a minimum when considered as a function of b, the oscillator size parameter. These results suggest that further efforts in the direction of obtaining simultaneous self-consistency for the wave functions *and* energy denominators might yield interesting results.

Ideally, the spectral corrections should be made for the calculations reported in Table II. It is expected that this correction to the binding energy would be about $+1$ MeV per particle for the two smaller values of b and slightly less than 1 MeV for the larger values of b. Generally, this correction will reduce the sensitivity of the calculated binding energy to the choice of the oscillator parameter. When several oscillator functions are used to expand each orbital (as in the calculations of Table II), the spectral correction may be most readily evaluated in perturbation theory, the perturbation involving the matrix elements of

$$v_T^{\mathrm{OD}}\left(\frac{Q}{e_{\mathrm{HF}}}-\frac{Q}{e(\Delta)}\right)v_T^{\mathrm{OD}},$$

where $e(\Delta)$ is the energy denominator used in this work and e_{HF} would be the energy denominator constructed using the single-particle energies obtained from the Hartree-Fock calculation. The expansion coefficients

TABLE VII. Calculated properties of Ca^{40}. (Second-order terms in VP not included. Three oscillator functions were used for each orbital.)

b (F)	1.76	2.09	2.17	Experimental
Single-particle energies (MeV)				
$0s_{1/2}$	−74.3	−74.8	−69.7	
$0p_{3/2}$	−47.5	−48.4	−44.9	
$0p_{1/2}$	−42.3	−43.5	−40.6	
$0d_{5/2}$	−22.7	−22.8	−21.7	−22.8 (neutron)[a]
$1s_{1/2}$	−17.3	−17.6	−15.3	−18.4 (neutron)[a]
$0d_{3/2}$	−14.4	−15.9	−14.4	−15.8 (neutron)[a]
B. E./A (MeV)	−5.73	−6.30	−5.49	
E_{Coul}/A (MeV)	1.85	1.85	1.85	
$E_{\mathrm{c.m.}}/A$ (MeV)	+0.26	+0.26	+0.26	
B. E./A (MeV) (including Coulomb and c.m. corrections)	−4.14	−4.71	−3.90	−8.55
$0p_{3/2}-0p_{1/2}$ splitting (MeV)	5.2	4.9	4.3	
$0d_{5/2}-0d_{3/2}$ splitting (MeV)	8.3	7.9	7.3	7.0[a]
Rms radius (F)	2.97	2.99	3.08	3.52[b]

[a] B. L. Cohen, Phys. Rev. **130**, 227 (1963).
[b] R. Hofstader, Ann. Rev. Nucl. Sci. **7**, 231 (1957).

TABLE VIII. Calculated properties of Ca^{40}. (Second-order terms in VP included only for relative matrix elements diagonal in the oscillator quantum number, n. Three oscillator functions were used for each orbital.)

b (F)	1.76	2.09	2.17	Experimental
Single-particle energies (MeV)				
$0s_{1/2}$	−85.7	−82.2	−76.9	
$0p_{3/2}$	−56.7	−54.3	−50.7	
$0p_{1/2}$	−52.4	−49.9	−46.4	
$0d_{5/2}$	−30.0	−28.1	−26.0	−22.8[a] (neutron)
$1s_{1/2}$	−26.7	−22.5	−19.9	−18.4 (neutron)
$0d_{3/2}$	−23.0	−20.4	−18.6	−15.8 (neutron)
B. E./A (MeV)	−10.03	−8.60	−7.62	
E_{Coul}/A (MeV)	1.85	1.85	1.85	
$E_{\text{c.m.}}/A$ (MeV)	+0.26	+0.26	+0.26	
B. E./A (MeV) (including Coulomb and c.m. corrections)	−8.44	−7.01	−6.03	−8.55
$0p_{3/2}-0p_{1/2}$ splitting (MeV)	4.3	4.4	4.3	
$0d_{5/2}-0d_{3/2}$ splitting (MeV)	7.0	7.7	7.4	7.0[a]
Rms radius (F)	2.96	2.95	3.03	3.52[b]

[a] B. L. Cohen, Phys. Rev. **130**, 227 (1963).

[b] R. Hofstader, Ann. Rev. Nucl. Sci. **7**, 231 (1957).

of the self-consistent orbitals in the harmonic-oscillator basis functions are presented in Table VI for the calculations reported in Tables I and II.

Similar calculations were carried out for Ca^{40} and the results obtained are presented in Tables VII–XI. For the calculations of Table VII the second-order terms in VP were not included. One finds reasonable values for the single-particle energies and spin-orbit splitting. The binding energies for rms radii are small compared to the corresponding experimental quantities. For the calculations reported in Table VIII the second-order terms in VP were included for the relative matrix elements diagonal in the oscillator quantum number n. The inclusion of these second-order terms leads to an increase in the binding of the single-particle orbitals and in the total binding energy. The spin-orbit splitting and rms radii are only slightly modified. Finally, a calculation was carried out with the second-order terms in VP included for relative matrix elements diagonal and nondiagonal in the oscillator quantum number n (see Table IX). The off-diagonal terms were included in the $^3P_0$, $^3P_1$, and $^1P_1$ states only. This approximation leads to a further increase in the single-particle energies, binding energies and spin-orbit splitting while the rms radii decrease with respect to the previous calculations. When compared to the experimental data the results are not satisfactory, particularly with respect to the small size obtained and the binding energy which is in excess of the experimental value. Again, these features may be improved through a better treatment of the energy denominators in the second-order terms.

Table X contains the results of calculations for Ca^{40}

TABLE IX. Calculated properties of Ca^{40}. (Second-order terms in VP included for relative matrix elements diagonal and non-diagonal in the oscillator quantum number n. Three oscillator functions were used for each orbital.)

b (F)	1.50	1.76	2.09	2.17	Experimental
Single-particle energies (MeV)					
$0s_{1/2}$	−101.9	−102.1	−90.0	−83.7	
$0p_{3/2}$	−67.0	−66.5	−59.8	−55.6	
$0p_{1/2}$	−59.5	−59.6	−54.9	−50.9	
$0d_{5/2}$	−35.5	−34.2	−31.3	−28.8	−22.8[a] (neutron)
$1s_{1/2}$	−30.6	−27.6	−23.7	−20.9	−18.4 (neutron)
$0d_{3/2}$	−24.1	−23.0	−22.6	−20.8	−15.8 (neutron)
B. E./A (MeV)	−10.93	−10.28	−9.52	−8.49	
E_{Coul}/A (MeV)	1.85	1.85	1.85	1.85	
$E_{\text{c.m.}}/A$ (MeV)	0.26	0.26	0.26	0.26	
B. E./A (MeV) (including Coulomb and c.m. corrections)	−9.34	−8.69	−7.93	−6.90	−8.55
$0p_{3/2}-0p_{1/2}$ splitting (MeV)	7.5	6.9	4.9	4.7	
$0d_{5/2}-0d_{3/2}$ splitting (MeV)	11.4	11.2	8.7	8.0	7.0[a]
Rms radius (F)	2.67	2.65	2.84	2.93	3.52[b]

[a] B. L. Cohen, Phys. Rev. **130**, 227 (1963).

[b] R. Hofstadter, Ann. Rev. Nucl. Sci. **7**, 231 (1957).

TABLE X. Single-particle energies and nuclear binding energy per particle for Ca^{40} (in MeV). The second-order terms were evaluated self-consistently as discussed in the text. A minimum number of oscillator functions were used.

	$\Delta=20$	Iteration (1)	(2)	(3)	(4)
$b=1.50$ F					
$0s_{1/2}$	−104.8	−84.0	−88.5	−87.6	−87.8
$0p_{3/2}$	−69.2	−58.1	−60.3	−59.9	−60.0
$0p_{1/2}$	−60.7	−50.6	−52.6	−52.2	−52.3
$0d_{5/2}$	−36.8	−31.6	−32.6	−32.4	−32.4
$1s_{1/2}$	−31.3	−25.3	−26.6	−26.3	−26.4
$0d_{3/2}$	−24.9	−19.6	−20.6	−20.4	−20.5
B.E./A^a	−10.83	−6.64	−7.54	−7.29	−7.40
$b=1.76$ F					
$0s_{1/2}$	−79.9	−68.4	−70.2	−69.9	−70.0
$0p_{3/2}$	−52.4	−46.4	−17.3	−47.2	−47.2
$0p_{1/2}$	−48.2	−42.5	−43.4	−43.3	−43.3
$0d_{5/2}$	−27.8	−25.0	−25.4	−25.4	−25.4
$1s_{1/2}$	−24.3	−21.1	−21.6	−21.5	−21.5
$0d_{3/2}$	−21.2	−18.8	−19.2	−19.1	−19.1
B.E./A^a	−9.11	−6.84	−7.19	−7.13	−7.15
$b=2.09$ F					
$0s_{1/2}$	−56.2	−51.0	−51.6	−51.5	−51.5
$0p_{3/2}$	−36.7	−34.1	−34.4	−34.3	−34.3
$0p_{1/2}$	−34.7	−32.2	−32.5	−32.5	−32.5
$0d_{5/2}$	−19.4	−18.3	−18.4	−18.4	−18.4
$1s_{1/2}$	−18.0	−16.6	−16.8	−16.8	−16.8
$0d_{3/2}$	−16.4	−15.4	−15.5	−15.5	−15.5
B.E./A^a	−6.55	−5.55	−5.66	−5.65	−5.65
$b=2.17$ F					
$0s_{1/2}$	−51.2	−47.0	−47.4	−47.3	−47.4
$0p_{3/2}$	−33.1	−31.0	−31.2	−31.2	−31.2
$0p_{1/2}$	−31.0	−29.0	−29.2	−29.2	−29.2
$0d_{5/2}$	−17.1	−16.3	−16.4	−16.4	−16.4
$1s_{1/2}$	−15.9	−14.9	−14.9	−14.9	−14.9
$0d_{3/2}$	−14.2	−13.5	−13.6	−13.5	−13.5
B.E./A^a	−5.59	−4.82	−4.90	−4.89	−4.89

[a] Uncorrected for center-of-mass or Coulomb energy.

similar to those reported in Table IV for the case of O^{16}. Again a degree of self-consistency was obtained for the energy denominators in the evaluation of the second-order tensor interaction in the $^3S_1$ state of relative motion. By comparing the single-particle energies reported in Table IX and the single-particle energies used in Table X for the minimum orbital calculation one may obtain a good idea of the spectral correction necessary for the results of Table IX. The spectral correction for $b=1.50$ and $b=1.76$ is thus expected to be about +3.4 MeV and for $b=2.17$ this correction will be about +2.0 MeV. Again, it appears that upon making the spectral correction for the results reported in Table IX the dependence of the calculated binding energy on the choice of the oscillator parameter will be reduced. In general, the results obtained with the approximations of this work do indicate that further efforts in the study of the properties of finite nuclei using realistic forces would be of interest. Comparison of the Yale potential with other realistic potentials provide an obvious extention of this work; however, it is also clear that a good treatment of the double self-consistency problem is the most desirable next step in studies of this kind.

TABLE XI. Correction to the Ca^{40} binding energy (in MeV).

b (F)	Binding energy/A for $\Delta=20$ (Table X)	Correction from using more orbitals (Table IX)	Spectral correction (Table X)	Total B.E./A^a
1.50	−10.83	−0.10	+3.43	−7.50
1.76	−9.11	−1.17	+1.96	−8.32
2.09	−6.55	−2.97	+0.90	−8.62
2.17	−5.59	−2.90	0.70	−7.79

[a] Uncorrected for center-of-mass and Coulomb energy.

Discussion

From the results of the calculations reported here it may be concluded that reasonable agreement with the ground-state properties of the nuclei O^{16} and Ca^{40} may be obtained starting from a "realistic" potential which provides a good fit to the nucleon-nucleon scattering data. It has been shown that the use of several oscillator functions in the expansion of the orbitals tends to reduce the dependence of the results upon the choice of the oscillator size parameter. The estimates given for the spectral corrections to the binding energy appear to justify a perturbative approach to these corrections and indicate that further work along these lines would be of interest. It would also be interesting to calculate the additional binding energy that would arise from the consideration of ground-state correlations due to vibrations about the spherical shape.

Finally, a calculation in which both the wave functions and energy denominations are given a self-consistent treatment would be highly desirable. Such a calculation would probably be necessary for a more accurate determination of the single-particle energies than that made here. It is well known that this form of double self-consistency is difficult to achieve and this feature remains an outstanding challenge for further calculations of this kind. Some discussion of this problem for finite nuclei appears in the work of Pal and Stamp.[10] These authors have carried through Hartree-Fock calculations for nonspherical nuclei using the effective interaction matrix elements derived from the Yale potential.

The work reported here may usefully be compared with the results of Hartree-Fock calculations which have been carried out with nonsingular forces. In particular, the nonlocal Tabakin potential[11] has been extensively investigated.[8] It has been found that with the inclusion of second-order terms the Tabakin potential is able to give a good account of the ground-

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[10] M. K. Pal and A. P. Stamp (to be published).

[11] F. Tabakin, Ann. Phys. (N. Y.) **30**, 51 (1964).

state properties of light nuclei[12] and application to the study of heavy nuclei is under way.

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APPENDIX

In the Appendix are presented tables of the effective interaction matrix elements used in this work. Table XII includes the contribution of the central $^3S_1$ potential and the second-order tensor terms. The second-order terms are evaluated with $k_F = 1.4\ \mathrm{F}^{-1}$ and $\Delta = 20$ MeV in the notation of I. For the central part of the interaction the use of a pseudopotential depending upon the number of nodes has led to an averaging of the off-diagonal elements and these average values are included in the table. In Table XIII second-order terms in the central pseudopotential for the $^3S_1$ state are presented. These are evaluated using plane-wave intermediate states as discussed in I. While the matrix elements given in Table XIII are not small, the convergence of the perturbation expansion in VP is good, the second-order terms being less than one-third of the first-order terms in VP.

TABLE XII. Relative matrix elements for the $^3S_1$ state of the Yale potential. The contribution of the terms $(v_l - VP)$ and $v_T{}^{\mathrm{OD}}(Q/e)v_T{}^{\mathrm{OD}}$ are included. The off-diagonal matrix elements of $(v_l - VP)$ have been averaged (see text), $b = (\hbar/M\omega)^{1/2}$ F.

n	n' \ b(F)	1.5	1.76	2.09	2.17	2.40
0	0	−10.6	−7.99	−5.57	−5.11	−4.02
	1	−7.92	−6.84	−5.29	−4.92	−4.04
	2	−4.69	−5.26	−4.54	−4.34	−3.70
	3	−1.81	−3.53	−3.77	−3.68	−4.28
	4	+0.63	−2.02	−2.96	−2.97	−2.8
	5	2.75	−0.65	−2.20	−2.29	−2.38
	6	4.34	+0.5	−1.45	−1.66	−1.96
1	1	−6.84	−6.40	−5.34	−5.01	−4.27
	2	−4.00	−5.05	−4.70	−4.54	−4.01
	3	−1.38	−3.41	−3.96	−3.90	−3.59
	4	+0.95	−1.91	−3.12	−3.159	−3.12
	5	+3.05	−0.50	−2.31	−2.43	−2.64
	6	4.64	+0.71	−1.51	−1.76	−2.18
2	2	−2.34	−4.21	−4.23	−4.22	−3.83
	3	−0.40	−2.84	−3.62	−3.69	−3.47
	4	1.46	−1.61	−2.86	−3.00	−3.04
	5	3.24	−0.27	−2.10	−2.32	−2.59
	6	4.62	+0.85	−1.33	−1.67	−2.13
3	3	0.74	−1.82	−3.15	−3.27	−3.19
	4	2.02	−0.82	−2.51	−2.69	−2.82
	5	3.36	+0.21	−1.86	−2.08	−2.41
	6	4.43	1.17	−1.15	−1.49	−1.99
4	4	2.68	−0.11	−2.00	−2.22	−2.51
	5	3.53	+0.66	−1.46	−1.70	−2.16
	6	4.24	1.41	−0.86	−1.19	−1.78
5	5	3.89	1.18	−1.04	−1.29	−1.86
	6	4.23	1.71	−0.54	−0.87	−1.54
6	6	4.21	2.03	−0.14	−0.53	−1.28

TABLE XIII. Second-order contribution $VP(Q/e)VP$ of the pseudopotential to the $^3S_1$ relative matrix elements for various values of $b = (\hbar/M\omega)^{1/2}$ F.

n	n' \ b(F)	1.50	1.76	2.09	2.17
0	0	−0.988	−0.606	−0.350	−0.318
1	1	−1.510	−0.947	−0.540	−0.498
2	2	−2.147	−1.191	−0.757	−0.639
3	3	−2.763	−1.632	−0.873	−0.753
4	4	−3.448	−1.954	−1.047	−0.925
5	5	−4.483	−2.339	−1.194	−1.083
6	6	−5.492	−2.718	−1.411	−1.217

In Table XIV results are presented for the $^3S_1$ matrix elements as a function of Δ. The column for $\Delta = 20$ corresponds to values reported in Table XII.

Table XV contains the matrix element of the tensor potential coupling the $^3S_1$ states to the $^3D_1$ states. Table XVI contains the matrix elements of $(v^l - VP)$ for the

TABLE XIV. Relative matrix elements for the $^3S_1$ state of the Yale potential for various values of Δ. The contribution of the terms $(v_l - VP)$ and $V_T{}^{\mathrm{OD}}(Q/e)v_T{}^{\mathrm{OD}}$ are included.

		Δ (MeV)				
		20	70	120	170	220
$b = 1.50$ F						
n	n'					
0	0	−10.61	−8.41	−7.28	−6.41	−5.70
1	1	−6.84	−4.67	−3.63	−2.80	−1.07
2	2	−2.34	−0.86	−0.05	0.60	
3	3	0.74	+1.77	2.34	2.82	3.22
$b = 1.76$ F						
n	n'					
0	0	−7.99	−6.44	−5.65	−5.04	−4.56
1	1	−6.40	−4.80	−3.96	−3.31	−2.78
2	2	−4.21	−2.84	−2.11	−1.53	−1.05
3	3	−1.82	−0.72	−0.12	0.37	0.77
$b = 2.09$ F						
n	n'					
0	0	−5.57	−4.47	−3.95	−3.56	−3.24
1	1	−5.34	−4.17	−3.56	−3.09	−2.71
2	2	−4.23	−3.10	−2.50	−2.05	−1.66
3	3	−3.15	−2.14	−1.61	−1.17	−0.84
$b = 2.17$ F						
n	n'					
0	0	−5.11	−3.99	−3.52	−3.35	−3.07
1	1	−5.01	−3.92	−3.36	−2.32	−1.98
2	2	−4.22	−3.15	−2.59	−2.16	−1.81
3	3	−3.27	−2.30	−1.79	−1.39	−1.06

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[12] W. Bassichis and A. K. Kerman (to be published); M. K. Pal, J. P. Svenne and A. K. Kerman, in *Proceedings of the International Conference on Nuclear Physics, Gatlinburg, Tennessee, 1966* (Oak Ridge National Laboratory, Oak Ridge, Tennessee, 1966), Paper 6.23, p. 64.

TABLE XV. Matrix elements of the tensor potential between the correlated $^3S_1$ and $^3D_1$ states. The quantum number n refers to the $^3S_1$ state and n' refers to the $^3D_1$ state. [$b=(\hbar/M\omega)^{1/2}$ F]

n	n' \ b(F)	1.5	1.76	2.09	2.17	2.40
0	0	−9.21	−5.50	−3.07	−2.70	−1.89
	1	−12.5	−7.74	−4.47	−3.95	−2.82
	2	−14.49	−9.13	−5.40	−4.80	−3.47
	3	−15.6	−10.0	−6.06	−5.41	−3.96
	4	−16.2	−10.6	−6.54	−5.86	−4.32
	5	−16.6	−11.0	−6.89	−6.19	−4.61
	6	−16.7	−11.3	−7.15	−6.44	−4.83
1	0	−4.16	−2.85	−1.81	−1.63	−1.22
	1	−8.49	−5.50	−3.34	−2.98	−2.19
	2	−11.6	−7.54	−4.59	−4.10	−3.01
	3	−13.7	−9.04	−5.56	−4.98	−3.68
	4	−15.2	−10.1	−6.31	−5.66	−4.21
	5	−16.1	−10.9	−6.89	−6.20	−4.64
	6	−16.7	−11.4	−7.34	−6.62	−4.98
2	0	−2.02	−1.57	−1.10	−1.01	−0.79
	1	−4.56	−3.32	−2.23	−2.03	−1.56
	2	−7.62	−5.28	−3.41	−3.08	−2.33
	3	−10.2	−7.01	−4.48	−4.04	−3.04
	4	−12.2	−8.41	−5.37	−4.86	−3.66
	5	−13.7	−9.49	−6.13	−5.54	−4.18
	6	−14.7	−10.3	−6.73	−6.09	−4.62
3	0	−0.98	−0.92	−0.72	−0.67	−0.55
	1	−2.33	−2.00	−1.48	−1.37	−1.10
	2	−4.28	−3.40	−2.40	−2.20	−1.73
	3	−6.61	−4.95	−3.37	−3.07	−2.38
	4	−8.75	−6.42	−4.29	−3.90	−3.00
	5	−10.5	−7.68	−5.11	−4.64	−3.87
	6	−11.93	−8.71	−5.81	−5.29	−4.07
4	0	−0.40	−0.54	−0.48	−0.46	−0.39
	1	−1.06	−1.20	−1.00	−0.95	−0.79
	2	−2.13	−2.10	−1.67	−1.56	−1.28
	3	−3.68	−3.25	−2.44	−2.27	−1.82
	4	−5.52	−4.53	−3.26	−3.01	−2.39
	5	−7.32	−5.77	−4.07	−3.73	−2.94
	6	−8.88	−6.89	−4.81	−4.41	−3.45
5	0	−0.05	−0.30	−0.33	−0.32	−0.29
	1	−0.30	−0.69	−0.69	−0.67	−0.58
	2	−0.83	−1.25	−1.16	−1.11	−0.95
	3	−1.69	−2.02	−1.73	−1.64	−1.38
	4	−2.95	−2.98	−2.40	−2.25	−1.86
	5	−4.45	−4.05	−3.11	−2.90	−2.35
	6	−5.97	−5.12	−3.82	−3.54	−2.84
6	0	+0.18	−0.13	−0.22	−0.22	−0.21
	1	+0.19	−0.34	−0.47	−0.47	−0.44
	2	+0.02	−0.67	−0.80	−0.79	−0.71
	3	−0.38	−1.15	−1.22	−1.18	−1.04
	4	−1.09	−1.80	−1.73	−1.65	−1.43
	5	−2.12	−2.62	−2.31	−2.19	−1.85
	6	−3.36	−3.52	−2.93	−2.76	−2.29

$^1S_0$ state, the off-diagonal elements again representing an averaged value. Table XVII contains some of the second-order terms for the $^1S_0$ pseudopotential. Tables XVIII–XXVIII contain the matrix elements of (v_l-VP) for the P and D state used in these calculations. For those states for which the second-order terms in VP are significant ($^1P_1$,$^3P_0$,$^3P_1$), tables of the matrix elements of the quantity $(v_l-VP)+VP(Q/e)VP$ are included. All the reported matrix elements are given in MeV.

TABLE XVI. Matrix elements of (v_l-VP) for the $^1S_0$ potential for various values of b. The off-diagonal matrix elements of (v_l-VP) have been averaged. [$b=\hbar/M\omega)^{1/2}$ F]

n	n' \ b(F)	1.50	1.76	2.09	2.17	2.40
0	0	−7.80	−5.96	−4.23	−3.88	−3.07
	1	−4.93	−4.59	−3.75	−3.18	−2.00
	2	−2.16	−3.11	−2.94	−2.84	−2.55
	3	−0.33	−2.62	−2.24	−2.19	−2.11
	4	2.59	−0.20	−1.43	−1.53	−1.69
	5	4.34	0.98	−0.81	−0.93	−1.27
	6	5.61	2.98	−0.12	−0.37	−0.99
1	1	−3.53	−3.90	−3.59	−3.33	−2.89
	2	−1.43	−2.72	−2.90	−2.82	−2.61
	3	0.97	−1.35	−2.24	−2.41	−2.16
	4	2.83	0.03	−1.42	−1.76	−1.76
	5	4.60	1.23		−0.89	−1.33
	6	5.88	2.64	−0.05	−0.61	−0.86
2	2	−0.25	−1.98	−2.39	−2.43	−2.44
	3	2.51	−0.91	−2.37	−1.92	−3.06
	4	3.03	0.29	−1.14	−1.33	−1.70
	5	4.50	1.85	−0.57	−0.99	−1.29
	6	5.64	2.31	−0.12	−0.18	−0.88
3	3	2.52	−0.18	−1.49	−1.53	−1.75
	4	3.48	0.76	−0.88	−1.00	−1.46
	5	4.53	1.61	−0.40	−0.54	−1.10
	6	5.39	2.41	0.23	−0.03	−0.68
4	4	3.90	1.36	−0.41	−0.67	−1.22
	5	4.51	1.98	0.15	−0.25	−0.92
	6	5.06	2.09	0.50	0.27	−0.54
5	5	4.68	2.38	0.26	0.07	−0.66
	6	4.90	2.79	0.69	0.42	−0.35
6	6	4.82	3.00	1.00	0.89	−0.08

TABLE XVII. Second-order contribution [$VP(Q/e)VP$] of the pseudopotential for the $^1S_0$ relative matrix element for various values of b.

n	n' \ b(F)	1.50	1.76	2.09	2.17
0	0	−0.195	−0.136	−0.082	−0.079
1	1	−0.201	−0.144	−0.102	−0.094
2	2	−0.290	−0.157	−0.103	−0.096
3	3	−0.536	−0.214	−0.109	−0.097
4	4	−0.954	−0.319	−0.129	−0.110
5	5	−1.640	−0.525	−0.177	−0.140
6	6	−2.584	−0.800	−0.237	−0.190

TABLE XVIII. Matrix elements of $(v_l - VP)$ for the $^1P_1$ potential for various values of b.

n	$n' \backslash b$(F)	1.50	1.76	2.09	2.17	2.40
0	0	4.61	2.49	1.28	1.12	0.77
	1	5.80	2.99	1.53	1.38	0.91
	2	7.00	3.45	1.68	1.45	0.97
	3	7.62	4.02	1.87	1.60	1.04
	4	8.26	4.33	2.01	1.72	1.13
	5	8.95	4.56	2.23	1.95	1.20
	6	8.92	4.86	2.40	2.06	1.27
1	1	8.41	4.36	2.19	1.88	1.27
	2	10.29	5.20	2.56	2.20	1.47
	3	11.14	6.06	2.87	2.47	1.61
	4	11.9	6.48	3.09	2.66	1.76
	5	12.9	6.79	3.48	2.99	1.87
	6	12.8	7.21	3.66	3.15	1.97
2	2	12.4	6.40	3.16	2.73	1.81
	3	13.5	7.57	3.65	3.14	2.05
	4	14.5	8.10	3.95	3.41	2.27
	5	15.6	8.47	4.44	3.83	2.42
	6	15.5	8.97	4.65	4.02	2.55
3	3	15.0	8.63	4.22	3.63	2.38
	4	16.2	9.32	4.63	4.00	2.68
	5	17.5	9.76	5.23	4.52	2.88
	6	17.3	10.3	5.48	4.75	3.04
4	4	17.2	10.1	5.15	4.46	3.00
	5	18.6	10.7	5.85	5.08	3.25
	6	18.5	11.3	6.15	5.36	3.45
5	5	19.1	11.3	6.34	5.52	3.55
	6	19.1	12.0	6.69	5.85	3.79
6	6	19.1	12.5	7.10	5.52	4.07

TABLE XIX. Matrix elements for the $^1P_1$ potential for various values of b. The table includes the matrix elements of $(v_l - VP) + VP(Q/e)VP$.

n	$n' \backslash b$(F)	1.50	1.76	2.09	2.17
0	0	2.598	1.522	0.853	0.758
	1	2.853	1.543	0.872	0.774
	2	2.315	1.636	0.845	0.741
	3	2.359	1.292	0.884	0.770
	4	2.609	1.316	0.906	0.785
	5	3.087	1.334	0.695	0.602
	6	2.980	1.480	0.716	0.612
1	1	4.103	2.190	1.188	1.043
	2	3.445	2.492	1.286	1.127
	3	3.448	1.979	1.376	1.200
	4	3.737	1.982	1.468	1.224
	5	4.376	1.976	1.076	0.939
	6	4.209	2.168	1.082	0.944
2	2	4.067	3.009	1.541	1.345
	3	3.774	2.474	1.741	1.517
	4	4.086	2.480	1.809	1.576
	5	5.220	2.456	1.386	1.217
	6	4.989	2.671	1.382	1.214
3	3	4.512	2.749	1.975	1.723
	4	4.964	2.839	2.137	1.842
	5	5.765	2.822	1.633	1.439
	6	5.478	3.046	1.632	1.441
4	4	5.130	3.019	2.287	2.020
	5	6.049	3.058	1.799	1.600
	6	5.771	3.332	1.728	1.688
5	5	6.069	3.161	1.917	1.700
	6	5.856	3.490	1.965	1.749
6	6	5.720	3.580	2.041	1.115

TABLE XX. Matrix elements of $(v_l - VP)$ for the $^3P_0$ potential for various values of b.

n	$n' \backslash b$(F)	1.50	1.76	2.09	2.17	2.40
0	0	−2.84	−2.16	−1.44	−1.30	−0.97
	1	−1.01	−1.39	−1.21	−1.14	−0.92
	2	0.65	−0.50	−0.80	−0.80	−0.74
	3	2.08	0.27	−0.40	−0.47	−0.52
	4	2.92	0.88	−0.06	−0.16	−0.33
	5	3.70	1.43	0.23	0.10	−0.14
	6	4.32	1.81	0.48	0.33	0.02
1	1	−0.52	−1.26	−1.27	−1.22	−1.04
	2	0.98	−0.49	−0.94	−0.95	−0.92
	3	2.73	0.39	−0.50	−0.60	−0.68
	4	3.90	1.19	−0.09	−0.22	−0.44
	5	5.02	1.96	0.32	0.14	−0.20
	6	5.96	2.52	0.67	0.45	0.02
2	2	1.70	−0.10	−0.79	−0.83	−0.88
	3	3.24	0.63	−0.44	−0.56	−0.69
	4	4.49	1.42	−0.04	−0.20	−0.47
	5	5.70	2.29	0.40	0.19	−0.22
	6	6.85	2.94	0.80	0.55	0.04
3	3	3.89	1.07	−0.22	−0.38	−0.59
	4	4.89	1.71	0.09	−0.08	−0.41
	5	6.07	2.55	0.51	0.28	−0.18
	6	7.28	3.22	0.92	0.64	0.08
4	4	5.35	2.10	0.32	0.11	−0.28
	5	6.31	2.82	0.68	0.43	−0.09
	6	7.45	3.44	1.06	0.76	0.15
5	5	6.56	3.15	0.90	0.63	0.04
	6	7.50	3.66	1.23	0.92	0.23
6	6	7.53	3.91	1.43	1.11	0.40

TABLE XXI. Matrix elements for the $^3P_0$ potential for various values of b. The table includes the matrix elements of $(v_l - VP) + VP(Q/e)VP$.

n	$n' \backslash b$(F)	1.50	1.76	2.09	2.17
0	0	−3.242	−2.361	−1.504	−1.353
	1	−1.605	−2.681	−1.344	−1.249
	2	−0.063	−0.863	−0.967	−0.941
	3	1.073	−0.140	−0.602	−0.636
	4	1.882	0.427	−0.289	−0.355
	5	2.580	0.816	−0.004	−0.100
	6	2.868	1.164	−0.230	0.112
1	1	−1.385	−1.691	−1.565	−1.389
	2	−0.962	−1.063	−1.198	−1.169
	3	1.255	−0.227	−0.807	−0.853
	4	2.374	0.500	−0.428	−0.510
	5	3.373	1.037	−0.047	−0.196
	6	4.290	1.549	0.282	0.028
2	2	0.420	−0.779	−1.113	−1.110
	3	1.437	−0.143	−0.823	−0.884
	4	2.587	0.564	−0.473	−0.566
	5	3.689	1.133	−0.067	−0.209
	6	4.804	1.741	0.307	0.124
3	3	1.848	0.165	−0.670	−0.762
	4	2.708	0.713	−0.408	−0.515
	5	3.796	1.214	−0.037	−0.190
	6	4.975	1.805	0.335	0.140
4	4	3.002	0.995	−0.242	−0.376
	5	3.867	1.351	0.063	−0.102
	6	4.973	1.899	0.395	0.194
5	5	4.018	1.573	0.227	0.046
	6	4.928	2.008	0.502	0.292
6	6	4.921	2.175	0.658	0.433

TABLE XXII. Matrix elements of (v_l-VP) for the $^3P_1$ potential for various values of b.

	b(F)	1.50	1.76	2.09	2.17	2.40
n	n'					
0	0	4.43	2.62	1.45	1.27	0.89
	1	4.62	2.80	1.60	1.42	1.01
	2	4.56	2.73	1.60	1.42	1.02
	3	4.52	2.66	1.56	1.33	1.01
	4	4.40	2.69	1.53	1.34	0.98
	5	4.50	2.60	1.49	1.32	0.96
	6	4.48	2.56	1.50	1.24	0.94
1	1	6.05	3.65	2.08	1.84	1.32
	2	6.49	3.88	2.22	2.00	1.44
	3	6.62	3.92	2.28	2.06	1.48
	4	6.53	4.03	2.29	2.01	1.46
	5	6.68	3.92	2.27	2.00	1.45
	6	6.63	3.88	2.30	2.98	1.44
2	2	7.43	4.46	2.59	2.30	1.65
	3	7.95	4.77	2.75	2.43	1.77
	4	7.99	4.98	2.83	2.43	1.81
	5	8.23	4.91	2.83	2.51	1.82
	6	8.18	4.88	2.91	2.51	1.83
3	3	3.61	5.17	3.02	2.67	1.95
	4	8.91	5.62	3.20	2.81	2.04
	5	9.29	5.68	3.28	2.90	2.10
	6	9.29	5.66	3.40	2.43	2.13
4	4	9.32	5.98	3.43	3.01	2.19
	5	9.91	6.11	3.59	3.17	2.29
	6	10.01	6.22	3.77	3.25	2.37
5	5	10.1	6.37	3.78	3.34	2.42
	6	10.3	6.58	4.03	3.48	2.54
6	6	10.3	6.75	4.20	3.62	2.66

TABLE XXIII. Matrix elements for the $^3P_1$ potential. The table includes the matrix elements of $(v_l-VP)+VP(Q/e)VP$.

	b(F)	1.50	1.76	2.09	2.17
n	n'				
0	0	4.007	2.416	.1.389	1.221
	1	4.001	2.494	1.466	1.304
	2	3.797	2.414	1.428	1.278
	3	3.434	2.222	1.354	1.210
	4	3.250	2.081	1.294	1.147
	5	3.249	1.942	1.231	1.102
	6	3.259	1.875	1.162	1.061
1	1	5.139	3.190	1.874	1.668
	2	5.367	3.305	1.956	1.778
	3	5.050	3.258	1.971	1.756
	4	4.935	3.113	1.931	1.707
	5	4.916	3.002	1.897	1.666
	6	4.848	2.847	1.775	1.621
2	2	6.065	3.741	2.253	2.016
	3	6.029	3.900	2.353	2.093
	4	5.926	3.748	2.378	2.100
	5	6.077	3.676	2.335	2.089
	6	6.004	3.594	2.247	2.054
3	3	6.443	4.190	2.550	2.269
	4	6.582	4.298	2.668	2.354
	5	5.803	4.109	2.700	2.395
	6	6.835	4.163	2.615	2.390
4	4	6.814	4.515	2.825	2.493
	5	7.308	4.541	2.931	2.600
	6	7.346	4.569	2.886	2.640
5	5	7.396	4.683	3.058	2.715
	6	7.609	4.811	3.062	2.807
6	6	7.551	4.904	3.159	2.901

TABLE XXIV. Matrix elements of v_l for the $^3P_2$ state for various values of b. $(VP=0.)$

	b(F)	1.50	1.76	2.09	2.17	2.40
n	n'					
0	0	−1.56	−0.83	−0.40	−0.34	−0.22
	1	−1.88	−1.06	−0.54	−0.46	−0.31
	2	−1.93	−1.14	−0.61	−0.53	−0.36
	3	−1.82	−1.15	−0.64	−0.56	−0.39
	4	−1.62	−1.11	−0.66	−0.57	−0.40
	5	−1.35	−1.04	−0.65	−0.57	−0.41
	6	−1.05	−0.96	−0.63	−0.57	−0.41
1	1	−2.46	−1.42	−0.75	−0.65	−0.44
	2	−2.61	−1.59	−0.87	−0.75	−0.51
	3	−2.52	−1.63	−0.93	−0.81	−0.56
	4	−2.28	−1.59	−0.96	−0.84	−0.59
	5	−1.91	−1.50	−0.95	−0.84	−0.61
	6	−1.50	−1.39	−0.93	−0.84	−0.62
2	2	−2.93	−1.84	−1.03	−0.90	−0.62
	3	−2.88	−1.91	−1.11	−0.98	−0.69
	4	−2.64	−1.89	−1.16	−1.02	−0.72
	5	−2.24	−1.81	−1.17	−1.04	−0.76
	6	−1.78	−1.69	−1.14	−1.04	−0.77
3	3	−3.03	−2.07	−1.24	−1.09	−0.77
	4	−2.81	−2.07	−1.30	−1.15	−0.82
	5	−2.41	−2.00	−1.32	−1.18	−0.87
	6	−1.93	−1.88	−1.30	−1.18	−0.88
4	4	−2.83	−2.17	−1.40	−1.24	−0.92
	5	−2.45	−2.11	−1.43	−1.27	−0.95
	6	−1.98	−2.00	−1.41	−1.29	−0.97
5	5	−2.40	−2.15	−1.49	−1.34	−1.01
	6	−1.95	−2.05	−1.48	−1.36	−1.04
6	6	−1.86	−2.05	−1.52	−1.41	−1.09

TABLE XXV. Matrix elements of v_l for the $^1D_2$ state for various values of b. $(VP=0.)$

	b(F)	1.50	1.76	2.09	2.17	2.40
n	n'					
0	0	−1.11	−0.58	−0.37	−0.23	−0.15
	1	−1.11	−0.65	−0.38	−0.27	−0.13
	2	−1.13	−0.64	−0.33	−0.28	−0.18
	3	−1.02	−0.61	−0.32	−0.28	−0.19
	4	−0.90	−0.56	−0.31	−0.27	−0.18
	5	−0.78	−0.51	−0.29	−0.26	−0.18
	6	−0.67	−0.46	−0.28	−0.24	−0.17
1	1	−1.66	−0.91	−0.46	−0.39	−0.25
	2	−1.73	−0.99	−0.51	−0.44	−0.29
	3	−1.64	−0.98	−0.53	−0.46	−0.31
	4	−1.50	−0.93	−0.52	−0.45	−0.31
	5	−1.34	−0.87	−0.50	−0.44	−0.30
	6	−1.17	−0.81	−0.48	−0.42	−0.30
2	2	−2.05	−1.18	−0.63	−0.54	−0.36
	3	−2.07	−1.25	−0.68	−0.59	−0.40
	4	−1.97	−1.23	−0.69	−0.60	−0.41
	5	−1.80	−1.18	−0.68	−0.60	−0.41
	6	−1.60	−1.11	−0.66	−0.58	−0.41
3	3	−2.27	−1.40	−0.77	−0.67	−0.46
	4	−2.28	−1.44	−0.81	−0.71	−0.49
	5	−2.15	−1.41	−0.82	−0.72	−0.50
	6	−1.96	−1.35	−0.81	−0.72	−0.51
4	4	−2.41	−1.55	−0.89	−0.78	−0.54
	5	−2.37	−1.58	−0.92	−0.82	−0.57
	6	−2.23	−1.55	−0.93	−0.82	−0.58
5	5	−2.46	−1.66	−0.99	−0.87	−0.62
	6	−2.38	−1.67	−1.02	−0.90	−0.64
6	6	−2.42	−1.73	−1.07	−0.95	−0.68

TABLE XXVI. Matrix elements of $(v_l - VP)$ for the ${}^3D_1$ state for various values of b.

n	n' ╲ b(F)	1.50	1.76	2.09	2.17	2.40
0	0	1.90	1.08	0.50	0.48	0.31
	1	1.72	1.06	0.59	0.52	0.36
	2	1.40	0.91	0.54	0.48	0.34
	3	1.11	0.77	0.48	0.43	0.31
	4	0.87	0.64	0.42	0.38	0.28
	5	0.69	0.53	0.36	0.33	0.25
	6	0.54	0.44	0.31	0.29	0.23
1	1	2.30	1.42	0.80	0.70	0.49
	2	2.18	1.41	0.83	0.74	0.52
	3	1.86	1.27	0.79	0.70	0.51
	4	1.53	1.10	0.71	0.64	0.48
	5	1.25	0.94	0.63	0.58	0.44
	6	1.00	0.80	0.56	0.51	0.40
2	2	2.50	1.62	0.97	0.86	0.62
	3	2.38	1.61	0.99	0.88	0.64
	4	2.09	1.48	0.95	0.85	0.63
	5	1.77	1.31	0.87	0.79	0.60
	6	1.46	1.14	0.79	0.72	0.56
3	3	2.57	1.75	1.09	0.97	0.71
	4	2.46	1.72	1.10	0.99	0.73
	5	2.19	1.60	1.06	0.96	0.72
	6	1.88	1.44	0.99	0.90	0.69
4	4	2.57	1.82	1.17	1.06	0.79
	5	2.46	1.79	1.18	1.07	0.80
	6	2.22	1.67	1.14	1.03	0.79
5	5	2.53	1.81	1.11	1.22	0.84
	6	2.42	1.76	1.11	1.22	0.85
6	6	2.45	1.79	1.14	1.25	0.88

TABLE XXVII. Matrix elements of $(v_l - VP)$ for the ${}^3D_2$ state for various values of b.

n	n' ╲ b(F)	1.50	1.76	2.09	2.17	2.40
0	0	−3.58	−2.01	−1.03	−0.39	−0.58
	1	−3.18	−1.98	−1.11	−0.97	−0.66
	2	−2.50	−1.70	−1.02	−0.90	−0.64
	3	−1.86	−1.40	−0.90	−0.81	−0.59
	4	−1.27	−1.13	−0.78	−0.71	−0.53
	5	−0.79	−0.89	−0.67	−0.62	−0.48
	6	−0.39	−0.66	−0.51	−0.53	−0.43
1	1	−4.16	−0.26	−1.49	−1.31	−0.90
	2	−3.78	−0.25	−1.55	−1.38	−0.98
	3	−3.02	−0.22	−1.46	−1.31	−0.96
	4	−2.16	−1.91	−1.32	−1.19	−0.90
	5	−1.41	−1.54	−1.15	−1.06	−0.82
	6	−0.70	−1.17	−1.00	−0.93	−0.74
2	2	−4.16	−2.93	−1.80	−1.60	−1.15
	3	−3.71	−2.82	−1.83	−1.64	−1.20
	4	−2.82	−2.50	−1.13	−1.57	−1.18
	5	−1.93	−2.09	−1.56	−1.43	−1.11
	6	−1.02	−1.66	−1.88	−1.29	−1.02
3	3	−3.76	−2.99	−1.99	−1.79	−1.33
	4	−3.10	−2.89	−1.99	−1.80	−1.36
	5	−2.26	−2.49	−1.87	−1.71	−1.33
	6	−1.24	−1.99	−1.70	−1.58	−1.26
4	4	−2.90	−2.87	−2.09	−1.90	−1.45
	5	−2.28	−2.67	−2.04	−1.88	−1.47
	6	−1.31	−2.22	−1.92	−1.79	−1.43
5	5	−1.93	−2.61	−2.09	−1.94	−1.54
	6	−1.14	−2.27	−2.04	−1.90	−1.54
6	6	−0.68	−2.14	−2.05	−1.93	−1.58

TABLE XXVIII. Matrix elements of $(v_l - VP)$ for the ${}^3D_3$ state for various values of b.

n	n' ╲ b(F)	1.50	1.76	2.09	2.17	2.40
0	0	0.14	0.05	0.01	0.01	0.01
	1	0.24	0.09	0.03	0.02	0.01
	2	0.32	0.12	0.04	0.03	0.02
	3	0.41	0.15	0.05	0.04	0.02
	4	0.48	0.18	0.06	0.05	0.02
	5	0.54	0.21	0.07	0.05	0.03
	6	0.59	0.24	0.08	0.06	0.04
1	1	0.40	0.15	0.05	0.04	0.02
	2	0.55	0.21	0.07	0.05	0.03
	3	0.71	0.27	0.09	0.07	0.04
	4	0.82	0.32	0.11	0.09	0.05
	5	0.94	0.38	0.13	0.10	0.06
	6	1.02	0.42	0.15	0.12	0.07
2	2	0.76	0.29	0.10	0.08	0.04
	3	0.98	0.38	0.13	0.10	0.06
	4	1.14	0.45	0.16	0.13	0.07
	5	1.30	0.53	0.19	0.15	0.08
	6	1.42	0.59	0.21	0.17	0.09
3	3	1.21	0.48	0.17	0.13	0.07
	4	1.42	0.57	0.21	0.16	0.09
	5	1.63	0.68	0.24	0.19	0.11
	6	1.78	0.76	0.27	0.22	0.12
4	4	1.66	0.68	0.25	0.20	0.11
	5	1.92	0.81	0.30	0.23	0.13
	6	2.09	0.91	0.33	0.27	0.15
5	5	2.16	0.91	0.35	0.27	0.15
	6	2.37	1.05	0.39	0.32	0.17
6	6	2.61	1.17	0.44	0.36	0.20