$1d_{3/2}$–$1f_{7/2}$ Energy Splitting at Ca^{40}†

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The low-lying levels of nuclei near closed shells are commonly assumed to be of pure, single-particle model configurations. On this basis the single-particle and single-hole energies used in shell-model calculations are taken from the experimental energy spectra of these nuclei. In recent years, however, both direct-reaction experiments and theoretical calculations have shown that there is considerable configuration mixing in the Ca^{40} ground-state wave function, associated with a depression in the ground-state energy. Since the underlying approximation is not valid, the use of experimental energy differences as the single-particle energies in shell-model calculations is not justified. From calculations of the effects of mixing on the $A=39$ and $A=41$ nuclei, as well as on Ca^{40}, it is found that the conventional experimental splittings overestimate the important $1d_{3/2}$-$1f_{7/2}$ energy difference by at least 1 MeV. A smaller error is contained in the "experimental" $2s_{1/2}$-$1f_{7/2}$ splitting. Similar effects occur in the oxygen region, but the overestimation in the $1p_{1/2}$-$1d_{5/2}$ splitting is much smaller, since the mixing is considerably less.

1. INTRODUCTION

We break a general shell-model matrix element into three terms. The first is the interaction among valence nucleons (including holes); the second is the interaction of the valence nucleons with the closed shells below the Fermi level; and the third is the interaction among nucleons of the closed shells. The absolute binding energies of nuclei are normally not considered in configuration-mixing calculations; thus, configuration-mixing calculations include only the first two terms, which involve valence nucleons.

The interaction of the valence nucleons with the closed shells of the core depends upon the single-particle quantum numbers only. One valence nucleon does not affect the interaction of another valence nucleon with the core. The binding energy of each nucleon is known as the "single-particle energy" for the nucleons in that valence shell.

The valence-valence interaction is a phenomenological two-body force, often called a "model" force. Since one is forced to carry out the calculation in a truncated basis and with simplified single-particle wave functions, one attempts to compensate for the inadequate basis by the use of an artificial force, generally stronger than the real nucleon-nucleon interaction. While this model force could be used to calculate single-particle energies, it is thought to be unwise to do so, because a model force cannot easily compensate for the differing errors of the valence-closed shell and valence-valence parts of the matrix element.

Since calculation of the single-particle energies from the model force used for the valence nucleons is undesirable, they must be determined in some other way. They can be regarded as parameters, which should be adjusted to give the best fit to the experimental data. More commonly, however, one makes assumptions which allow the single-particle energies to be extracted directly from experimental spectra. It is assumed that the extreme single-particle shell model[1] applies to the lowest states of nuclei both at and near the magic numbers. In this case the ground state of Ca^{40} is assumed to be a perfectly closed shell containing neither holes in the s-d shell nor particles in the p-f shell; the lowest $\frac{7}{2}^-$, $\frac{3}{2}^-$, $\frac{1}{2}^-$, and $\frac{5}{2}^-$ levels of Ca^{41} or Sc^{41} have a single nucleon in the $1f_{7/2}$, $2p_{3/2}$, $2p_{1/2}$, and $1f_{5/2}$ subshells outside the $A=40$ core; and the lowest $\frac{3}{2}^+$, $\frac{1}{2}^+$, and $\frac{5}{2}^+$ levels of K^{39} and Ca^{39} are the single $1d_{3/2}$, $2s_{1/2}$, and $1d_{5/2}$ hole configurations. With these assumptions, the binding energy of a $1f_{7/2}$ neutron about the $A=40$ core is taken to be the energy of the ground state of Ca^{41}, less the energy of the Ca^{40} ground state with a neutron at infinity. The other single-particle energies are determined in a similar way. This paper shows that these "experimental" single-particle energies in the Ca^{40} region are not literally correct.

That the extreme single-particle shell model for nuclei much removed from the magic numbers is defective, is well known. Recently, the breakdown of the model at the magic numbers, particularly in Ca^{40}, has

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[1] M. G. Mayer and J. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure* (John Wiley & Sons, Inc., New York, 1957).

been shown both experimentally[2] and theoretically.[3,4,5] This breakdown is in the form of appreciable admixtures in the Ca^{40} ground state of configurations of particles and holes, accompanied by a substantial depression in the ground-state energy. Since the approximation underlying the extraction of single-particle energies from experimental data is incorrect, the use of these experimental single-particle energies in shell-model calculations can only be justified on an *ad hoc* basis, by arguing that the use of a model force and the omission of higher configurations compensates for the errors in the single-particle energies. By our calculations, we show that the single-particle energies at the Ca^{40} closed shell, extracted in this way, differ from the exact single-particle energies by at least 1 MeV.

2. BASIC FORMALISM

In the usual shell-model notation of particles and holes,[6] a closed-shell configuration has diagonal binding energy E_0, a particle configuration has binding energy $E_0+\Delta_1(j_p)$, and a single-hole configuration has binding energy $E_0-\Delta_2(j_h)$. When excited configurations of nuclei are used in shell-model calculations, the particle and hole energies always appear as pairs $\Delta_1(j_p)-\Delta_2(j_h)$, called the single-particle level splittings. Both Δ_1 and Δ_2 normally are negative, and $|\Delta_2|>|\Delta_1|$, so that the splittings are positive. For Ca^{40}, the important $1d_{3/2}-1f_{7/2}$ splitting is

$$\Delta(1d_{3/2}-1f_{7/2})=\text{B.E.}[\psi(1d_{3/2}^{-1})]+\text{B.E.}[\psi(1f_{7/2}^{+1})]-2\,\text{B.E.}[\psi(0)].$$

The $2s_{1/2}-1f_{7/2}$ splitting is

$$\Delta(2s_{1/2}-1f_{7/2})=\text{B.E.}[\psi(2s_{1/2}^{-1})]+\text{B.E.}[\psi(1f_{7/2}^{+1})]-2\,\text{B.E.}[\psi(0)].$$

The assumptions involved in extracting the experimental single-particle energies are to equate their pure model configurations with low-lying states of actual nuclei

$$\text{B.E. }[\psi(1d_{3/2}^{-1})]\simeq\text{B.E. }(A=39,\text{ g.s.}),$$

$$\text{B.E. }[\psi(2s_{1/2}^{-1})]\simeq\text{B.E. }(A=39,\text{ lowest }\tfrac{1}{2}^+),$$

$$\text{B.E. }[\psi(0)]\simeq\text{B.E. }(\text{Ca}^{40},\text{ g.s.}),$$

and

$$\text{B.E. }[\psi(1f_{7/2}^{+1})]\simeq\text{B.E. }(A=41,\text{ g.s.}),$$

where g.s. indicates the ground state of the nucleus.

Thus, the experimental $d_{3/2}-f_{7/2}$ splitting is

$$\Delta_{\text{exp}}(d_{3/2}-f_{7/2})=\text{B.E. }(A=39,\text{ g.s.})+\text{B.E. }(A=41,\text{ g.s.})-2\text{B.E. }(\text{Ca}^{40},\text{ g.s.}).$$

From the experimental data on direct reactions, it is known that the wave functions of real nuclei depart from the pure-model configurations significantly.[2] Calculations on the ground-state mixing of Ca^{40} also bear out strong departures from pure configurations. The spherical calculations of Hubbard and Jolly[3] and the spherical-deformed calculations of Gerace and Green[4] both indicate that the Ca^{40} nucleus has a closed-shell configuration about 90% of the time, while the random-phase-approximation (RPA) calculation of Gillet and Sanderson[5] shows the ground state of Ca^{40} to be in the closed-shell configuration only about 30% of the time. For the spherical shell-model calculation, this divergence of the wave function from a pure single-particle configuration corresponds to a binding energy shift of 1–3 MeV.[7] A similar amount was obtained in the spherical-deformed study of Gerace.[8]

Mixing must depress all the ground states of the real nuclei to below the binding energies of the pure configurations. We define

$$\text{B.E. }[\psi(1d_{3/2}^{-1})]=\text{B.E. }(A=39,\text{ g.s.})+\delta_{3/2},$$

$$\text{B.E. }[\psi(2s_{1/2}^{-1})]=\text{B.E. }(A=39,\text{ lowest }\tfrac{1}{2}^+)+\delta_{1/2},$$

$$\text{B.E. }[\psi(0)]=\text{B.E. }(\text{Ca}^{40},\text{ g.s.})+\delta_0,$$

and

$$\text{B.E. }[\psi(1f_{7/2}^{+1})]=\text{B.E. }(A=41,\text{ g.s.})+\delta_{7/2}.$$

With these definitions, the exact single-particle splittings can be written as

$$\begin{aligned}\Delta_{\text{exact}}(d_{3/2}-f_{7/2})&=\text{B.E. }(A=39,\text{ g.s.})+\text{B.E. }(A=41,\text{ g.s.})-2\text{B.E. }(\text{Ca}^{40},\text{ g.s.})+\delta_{3/2}+\delta_{7/2}-2\delta_0\\&=\Delta_{\text{exp}}(d_{3/2}-f_{7/2})+\delta_{3/2}+\delta_{7/2}-2\delta_0,\end{aligned}$$

and

$$\Delta_{\text{exact}}(s_{1/2}-f_{7/2})=\Delta_{\text{exp}}(s_{1/2}-f_{7/2})+\delta_{1/2}+\delta_{7/2}-2\delta_0.$$

The δ's, which are always positive, represent the depression of the ground-state energy due to configuration mixing. Only if these depressions are all negligible or if it should happen that $\delta_{3/2}+\delta_{7/2}-2\delta_0\simeq\delta_{1/2}+\delta_{7/2}-2\delta_0\simeq 0$ will $\Delta_{\text{exp}}(d_{3/2}-f_{7/2})$ and $\Delta_{\text{exp}}(s_{1/2}-f_{7/2})$ agree wth the exact single-particle splittings. The $s_{1/2}-d_{3/2}$ experimental splitting will be correct if $\delta_{1/2}\simeq\delta_{3/2}$. In this work we calculate the values of the δ's in equivalent bases.

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[5] V. Gillet and E. A. Sanderson, Nucl. Phys. **A91**, 292 (1967).

[6] G. E. Brown, L. Castillejo, and J. A. Evans, Nucl. Phys. **22**, 1 (1961).

[7] L. B. Hubbard, thesis, M.I.T., 1967 (unpublished).

[8] W. J. Gerace, thesis, Princeton Univ., 1967 Technical Report PUC-937-264 (unpublished).

3. CALCULATIONS

To investigate the accuracy of the "experimental" single-particle splittings, we have completed configuration-mixing calulations for the following nuclear levels:

$A=39$, ground state ($\frac{3}{2}^+$),

$A=39$, lowest $\frac{1}{2}^+$,

$A=40$, ground state (0^+),

and

$A=41$, ground state ($\frac{7}{2}^-$).

For each of these levels, the basis states are the single-particle-model ground state and all states that can be made from the excited configuration constructed by adding two particles to the $1f_{7/2}$ shell of the single-particle ground state and removing two particles from the $1d_{3/2}$ shell (i.e., a two-particle, two-hole excitation is added to the single-particle-model state). These configurations are shown in Table I. The Hamiltonian has been diagonalized in a harmonic oscillator basis within these configurations.

These bases contain no components of spurious states. The one-hole, closed-shell, and one-particle states are completely nonspurious as only one L-S shell is filling at a time.[9] Each excited configuration is made by moving particles from the highest j-subshell below the Fermi level, to the lowest j-subshell above the Fermi level. Because of this procedure, the center of mass operator

$$\mathbf{R}=\sum_{i=1}^{A}\mathbf{r}_i/A$$

vanishes between the $2\hbar\omega$, two-particle, two-hole excitations of the bases and all $1\hbar\omega$, particle-hole excitations.[3] Thus, the excited configurations contain no spurious components.

The reduction of the many particle matrix element to a linear combination of two-particle matrix elements was done by the program PLEXUS, described elsewhere.[10]

We have tried two types of force. One is the "phenomenological" Gaussian force of Gillet and Sanderson[11] whose parameters ($W=0.175$, $M=0.575$, $H=0.100$, $B=0.250$; $V=-55$ MeV; $a/b=0.8$) are chosen to give a good RPA fit to the particle-hole states of Ca^{40}. The other is the nonlocal potential of Tabakin,[12] a realistic force whose parameters fit the nucleon-nucleon scattering data. Since the single-particle, harmonic-oscillator-well parameter $\gamma=m\omega/2\hbar$ is not well determined by the data, the Tabakin potential has been evaluated for a range of γ. Different kinds of realistic forces seem to

TABLE I. List of the basis configurations within which the Hamiltonian was diagonalized.

Nuclear Level	Basis configurations	Number of basis states
$A=39\ \frac{3}{2}^+$	$(d_{3/2})^{-1}$; $(d_{3/2})^{-3}(f_{7/2})^2$	17
$A=39\ \frac{1}{2}^+$	$(s_{1/2})^{-1}$; $(s_{1/2})^{-1}(d_{3/2})^{-2}(f_{7/2})^2$	18
$A=40\ 0^+$	0: $(d_{3/2})^{-2}(f_{7/2})^2$	5
$A=41\ \frac{7}{2}^-$	$(f_{7/2})^{+1}$; $(d_{3/2})^{-2}(f_{7/2})^3$	40

give near identical results in configuration-mixing calculations[7,13]; thus, the Tabakin potential may represent all realistic forces.

Both the phenomenological Gaussian force and the Tabakin force fail to split sufficiently the nuclear levels which would be degenerate in the single-particle model.[7] From this we conclude that both these forces are too weak at least in the usual particle-hole basis. For this reason we have used a stronger force, a variation of the Tabakin potential, which we call the "augmented" Tabakin force.[3] In the "augmented" force, the usual Tabakin matrix elements ($\gamma=3.5$) are uniformly increased by 1.356 to fit the separation of the lowest 3^- and 5^- levels of Ca^{40} in the usual particle-hole basis.

The only single-particle splitting used in this calculation is the $d_{3/2}$-$f_{7/2}$ splitting. We have tried two values, 7.04 MeV, which is near the "experimental" value, and 5.0 MeV, close to what we believe is actually the splitting. While the energy depressions do depend on the value used for the splitting, the variation turns out to be rather slow and a complete self-consistent calculation is unnecessary. The second splitting value is near the value 5.4 MeV preferred by Gerace and Green.[14]

Many configurations must mix into the ground state, and each of these must contribute to lowering the ground-state energies. The largest contribution to the ground-state depression is expected from the configuration constructed by moving two particles from the *highest* shell below the shell closure to the *lowest* shell above the closure. These configurations are our bases. Contributions from the excluded configurations are probably large; they are discussed in Sec. 4.

4. RESULTS

Results of the mixing calculation in the Ca^{40} region are given in Table II. Several forces and two $d_{3/2}-f_{7/2}$ splittings are shown. Although the various choices of parameters result in a wide spread in ground-state depressions, certain generalizations can be made. The effect of mixing the single-particle ground state and the

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[10] H. P. Jolly and L. B. Hubbard, MIT-LNS Report No. CTP 29, 1968 (unpublished).
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[14] W. J. Gerace and A. M. Green, Bull. Am. Phys. Soc. **12**, 585 (1967). W. J. Gerace and A. M. Green, Nucl. Phys. **A113**, 641 (1968).

TABLE II. Depressions $\delta_{1/2}$, $\delta_{3/2}$, δ_0, and $\delta_{7/2}$ of the lowest lying states in bases containing excited configurations made by adding $d_{3/2}^{-2}f_{7/2}^2$ to the single-particle-model lowest configurations.

$d_{3/2}$-$f_{7/2}$ splitting MeV	Force	$A=39$ $\frac{1}{2}^+$ MeV	$A=39$ $\frac{3}{2}^+$ MeV	$A=40$ 0^+ MeV	$A=41$ $\frac{7}{2}^-$ MeV	$\Delta_{exp}-\Delta_{exact}$ (MeV) $d_{3/2}$-$f_{7/2}$	$s_{1/2}$-$f_{7/2}$
7.04	Gaussian[a]	1.20	0.92	1.18	1.04	0.40	0.12
	Tabakin $\gamma=3.0$	2.18	1.56	2.09	1.54	1.08	0.46
	3.5	1.67	1.20	1.59	1.42	0.56	0.09
	4.0	1.30	0.94	1.23	1.11	0.41	0.05
5.0	Gaussian[a]	...	1.27	1.59	1.39	0.52	...
	Tabakin $\gamma=3.0$	2.64	1.90	2.53	2.01	1.15	0.41
	3.5	2.08	1.50	1.97	1.77	0.67	0.09
	4.0	1.66	1.20	1.56	1.41	0.51	0.05
	Tabakin augmented	3.33	2.41	3.15	2.84	1.05	0.13

[a] Parameters $a/b=0.8$; $W=0.175$, $M=0.575$, $H=0.100$, $B=0.250$; $V=-55$ MeV.

configuration with two particles promoted from the $d_{3/2}$ shell to the $f_{7/2}$ shell is to depress all the ground states by 1–3 MeV. These depressions are not equal. By our estimate, the greatest depression occurs for the lowest $\frac{1}{2}^+$ level of $A=39$. The Ca^{40} ground-state depression is almost as great. Both the $A=39$, $\frac{3}{2}^+$ depression and the $A=41$, $\frac{7}{2}^-$ depression are significantly less than the Ca^{40} depression.

The strength of the force has a large effect on these depressions. Both the ordinary Tabakin and the Gaussian forces are too weak to fit most of the experimental energy levels. For this reason we used the "augmented" Tabakin force, in which all matrix elements were multiplied by 1.356. This fits the splitting of the lowest 3^- and 5^- states of Ca^{40} in a particle-hole basis. While the force is arbitrary, we believe that the results should be close to those obtained with any reasonable force strong enough to fit the experimental spectra. The single-particle splitting used in the calculations also has an effect on the ground-state depression, increasing the depression as the splitting is reduced.

Since $\delta_{3/2}$ and $\delta_{7/2}$ are both smaller than δ_0, from the formula,

$$\Delta_{exact}(d_{3/2}-f_{7/2})=\Delta_{exp}(d_{3/2}-f_{7/2})+\delta_{3/2}+\delta_{7/2}-2\delta_0,$$

it can be seen that the experimental splitting overestimates the actual splitting in every case. This overestimate is not small; $2\delta_0-\delta_{3/2}-\delta_{7/2}$ is found to be between 0.35 and 1.15 MeV.

One can understand why the ground states depress unequally. For Ca^{40}, the two particles and two holes are coupled through four intermediate sets of T and J as $d_{3/2}^{-2}(TJ)$, $f_{7/2}^2(TJ)00$, but in the case of the configurations in which the ground state is not $T=0$ $J=0$, additional intermediate couplings may occur. For the $\frac{1}{2}^+$ states of $A=39$ there are 13 additional higher states mixing with the lowest state, as well as the four that are found for the 0^+ states of Ca^{40}. Because additional states are included, the energy depression of the lowest $A=39$, $\frac{1}{2}^+$ state should be more than for the lowest 0^+ state of $A=40$. The effect of this enhancement turns out to be small, on the order of 5% of the total depres-

TABLE III. Values of the splittings for the bases of Table I which yield the correct binding-energy differences.

	$d_{3/2}$-$f_{7/2}$ (MeV)	$s_{1/2}$-$f_{7/2}$ (MeV)
Gaussian	6.8	9.8
Tabakin $\gamma=3.0$	6.1	9.4
3.5	6.6	9.7
4.0	6.8	9.8
Tabakin augmented	6.2	9.7

TABLE IV. O^{16} ground-state depressions obtained by mixing configurations containing $p_{1/2}^{-2}d_{5/2}^{+2}$ with the ground states. All values are in MeV. The force parameters are taken from Gillet.[a]

	$A=15$ $\frac{1}{2}^-$	$A=16$ 0^+	$A=17$ $\frac{5}{2}^+$	$\Delta_{exp}-\Delta_{exact}$
Gaussian[a]				
$a/b=0.8$	0.095	0.191	0.123	0.164
0.9	0.156	0.307	0.203	0.255

[a] V. Gillet, thesis, University of Paris, 1962, Rapport No. 217, Centre d'Etudes Nucléares de Saclay, 1962 (unpublished); V. Gillet and N. Vinh Mau, Nucl. Phys. **54**, 321 (1964).

[b] O^{16} parameters are $W=0.35$, $M=0.35$, $H=0.40$, $B=-0.1$; $V=-40$ MeV.

sion, because the states corresponding to Ca^{40} are the most important ones.

In the case of the $A=39$, $\frac{3}{2}^+$ and $A=41$, $\frac{7}{2}^-$ levels, there are also more configurations than in the $A=40$, 0^+ situation, because here also there are more particles, and the over-all $J\neq 0$. At the same time, however, the Pauli principle acts between the existing $\frac{3}{2}^+$ hole or $\frac{7}{2}^-$ particle and the additional holes or particles in the same shell. The requirement for antisymmetry reduces the basis, both the important part which corresponds to the Ca^{40} basis and the additional states as well. For the $\frac{3}{2}^+$ situation, for example, one must take account of the fact that there are only five possible values of T and J for $(\frac{3}{2})^3TJ$, while for $(\frac{3}{2})^2\frac{3}{2}TJ$ with no antisymmetry requirement for the last $j=\frac{3}{2}$ particle there are 17 possible values of T and J. In a sense, a state like $(j_h)^{-1}$, $(j_h)^{-2}TJ(j_p)^2TJ$ only partially exists. In a proper (antisymmetric) basis, the number of states in the basis for $A=39$, $\frac{3}{2}^+$ and $A=41$, $\frac{7}{2}^-$ is still larger than the number in the basis for $A=40$, 0^+, but the mixing is not as strong, and the depression turns out to be substantially less. The "blocking" effect is more important than the enhancement provided by an additional particle.

These two effects either enhance the mixing or decrease it when there are quasiparticles in the ground state. Enhancement results when quasiparticles are in the ground state. Blocking arises when quasiparticles occupy shells which are also populated by the excitation. The effect of blocking is much greater than the effect of enhancement.

In these unequal depressions the lowest energy experimental splittings at closed shells are always bigger than the true splitting between the levels. From Table II, the overestimate we calculate for the $d_{3/2}$-$f_{7/2}$ splitting is between about 0.5 and 1.0 MeV. The $s_{1/2}$-$f_{7/2}$ splitting more nearly agrees with the experimental estimates, because there is both blocking from the $f_{7/2}$ particle and enhancement from the $s_{1/2}$ hole.

TABLE V. Depressions of ground state of Ca^{40} in MeV as a result of mixing in all states of the configurations $(s_{1/2}, d_{3/2})^{-2}f_{7/2}^2$.

Force	7.04 MeV $d_{3/2}$-$f_{7/2}$ splitting	5.0 MeV $d_{3/2}$-$f_{7/2}$ splitting
Gaussian[a]	1.49	1.98
Tabakin $\gamma=3.0$	2.50	3.01
3.5	1.92	2.37
4.0	1.50	1.89
Tabakin, augmented	···	8.81

[a] Parameters $a/b=0.8$, $W=0.175$, $M=0.575$, $H=0.100$, $B=0.250$; $V=-55$ MeV.

TABLE VI. Blocking and enhancement effects of various two-particle, two-hole excitations when added to the one quasiparticle configurations considered in this paper. SB = strong blocking, WB = weak blocking, and E = enhancement.

Excitation	Sum of experimental splittings	Nuclear levels $A=39$ $\frac{3}{2}^+$	$A=39$ $\frac{1}{2}^+$	$A=41$ $\frac{7}{2}^-$
$d_{3/2}^{-2}f_{7/2}^2$	14.1	SB	E	SB
$d_{3/2}^{-2}f_{7/2}p_{3/2}$	16.1	SB	E	WB
$s_{1/2}^{-1}d_{3/2}^{-1}f_{7/2}^2$	16.8	WB	WB	SB
$d_{3/2}^{-2}p_{3/2}^2$	18.0	SB	E	E
$d_{3/2}^{-2}f_{7/2}p_{1/2}$	18.1	SB	E	WB
$s_{1/2}^{-1}d_{3/2}^{-1}f_{7/2}p_{3/2}$	18.7	WB	WB	WB
$s_{1/2}^{-2}f_{7/2}^2$	19.6	E	SB	SB
$d_{3/2}^{-2}p_{3/2}p_{1/2}$	20.0	SB	E	E
$d_{3/2}^{-2}f_{7/2}f_{5/2}$	20.5	SB	E	WB
$s_{1/2}^{-1}d_{3/2}^{-1}p_{3/2}^2$	20.7	WB	WB	E
$s_{1/2}^{-1}d_{3/2}^{-1}f_{7/2}p_{1/2}$	20.8	WB	WB	WB

Since the blocking is stronger than the enhancement, the $s_{1/2}$-$f_{7/2}$ experimental splitting is still too great; but the error is only 10–40% of the $d_{3/2}$-$f_{7/2}$ overestimate

Assuming that the configurations used in our calculations are the important ones, the splitting can be adjusted to give the correct experimental binding energy differences. These values are shown in Table III.

Oxygen 16 and Calcium 40 are considered to have similar shell-model behavior arising from the closed-shell and self-conjugate properties ascribed to both. Since the shell model has been much more successful for O^{16} than it has been for Ca^{40}, one would expect O^{16} to be much closer to a true closed shell. We have tested the $p_{1/2}$-$d_{5/2}$ splitting in exactly the same way as the $d_{3/2}$-$f_{7/2}$ splitting for Ca^{40}. That is, the higher states that mix with the single-particle-model ground states for $A=15$, 16, and 17 are constructed from the configuration that adds two $p_{1/2}$ holes and two $d_{5/2}$ particles to the ground configurations. The results are shown in Table IV. The effects of blocking in the $A=15$ and 17 nuclei, analogous to the $A=39$ and 41 nuclei, are present, but the over-all mixing is much smaller. Thus, the amount of overestimation in the experimental splitting is calculated to be 1–2% for O^{16}, in contrast to the 5–15% found for Ca^{40}. The nucleus O^{16} is a much better approximation to a closed shell than Ca^{40}.

We have calculated only part of the Ca^{40} mixing, and for this reason splittings in Table III are not necessarily the exact values. For Ca^{40}, an additional calculation has been done with a larger basis, including all states of the configuration $(s_{1/2}, d_{3/2})^{-2}(f_{7/2})^2$. The results, assuming an $s_{1/2}$-$d_{3/2}$ splitting of 2.8 MeV, are given in Table V. The Ca^{40} 0^+ depression, in this basis

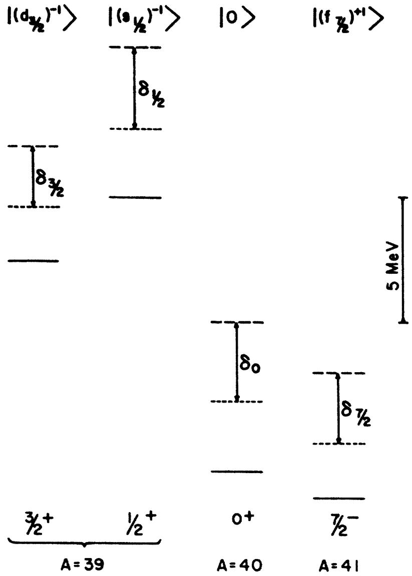

FIG. 1. The energy levels of interest in the Ca^{40} region are shown. The upper, dashed lines are the binding energies of the pure single-particle-model states whose labels are at the top. The δ's are the depressions calculated in our bases containing excited configuration with $d_{3/2}^{-2}f_{7/2}^{2}$ added to the single-particle-model ground states. The dotted lines are the levels obtained by mixing in these partial bases. The solid lines are the fully mixed results, the actual nuclear levels whose labels appear at the bottom. The energy differences between the dotted and solid lines are estimates based on qualitative arguments.

of nine states, is 20–25% greater than in the $(d_{3/2})^{-2}(f_{7/2})^{2}$ basis of five states (Table II). Thus, the $s_{1/2}$ contribution is substantial, and the $d_{5/2}$, $p_{3/2}$ and $f_{7/2}$ contributions are likely to be important as well.

To get an idea of the effects of the other excluded configurations, one must consider both the relative strength of the mixing of the additional states and the relative amounts of blocking and enhancement.

In Table VI, the blocking and enhancement for the eleven configurations whose experimental splittings are below 21 MeV are shown. "Strong" blocking occurs when two of the quasiparticles of the excitation are in the same shell as the ground configuration quasiparticle. If only one of the quasiparticles of the excitation is in the same shell as the single-particle-model ground-configuration quasiparticle, then "weak" blocking occurs. If the excitation quasiparticles are both in different shells from the ground-configuration quasiparticle, enhancement occurs. We have calculated two cases of strong blocking and one of enhancement. We suspect that weak blocking would have about the same magnitude as enhancement, but would have the opposite sign. The cutoff at 21 MeV is arbitrary, although the largest mixing components should be found for the configurations of Table VI.

For the $A=39$, $\frac{3}{2}^{+}$ states, there is strong blocking in over half of the configurations and enhancement in only one. For the $A=39$, $\frac{1}{2}^{+}$ level, however, six configurations have enhancement and strong blocking occurs in only one for $A=41$, $\frac{7}{2}^{-}$, there is weak blocking in five configurations, enhancement in three, and strong blocking in three. In a more complete basis we believe the $A=39$, $\frac{1}{2}^{+}$ will still depress slightly more than the $A=40$, 0^{+}; the $A=39$, $\frac{3}{2}^{+}$ ground state will depress 20–30% less than the $A=40$, 0^{+}; and the $A=41$, $\frac{7}{2}^{-}$ will depress perhaps 10% less than the $A=40$, 0^{+}. Thus, we estimate that the splittings should be

$$\Delta_{\rm exact}(s_{1/2}-f_{7/2})\simeq\Delta_{\rm exp}(s_{1/2}-f_{7/2})\simeq 10\ {\rm MeV},$$

and

$$\Delta_{\rm exact}(d_{3/2}-f_{7/2})\simeq\Delta_{\rm exp}(d_{3/2}-f_{7/2})-2\ {\rm MeV}\simeq 5\ {\rm MeV}.$$

This final estimate for the $d_{3/2}-f_{7/2}$ splitting corresponds closely with the estimates of Gerace and Green[14] and Hubbard.[7]

Our calculations and estimates are summarized in Fig. 1. While this graph is intended only to be schematic, when the energy scale is applied to it, it represents the proton levels as given by Endt and Van-der-Leun[15] and the calculated δ's obtained using the augmented Tabakin force. The total energy spread from the real nuclear levels to the pure-model configurations are our estimates.

5. CONCLUSIONS

The important $d_{3/2}$-$f_{7/2}$ splitting of the calcium region is significantly overestimated when it is taken from binding energy data. The exact value of this splitting should be significantly less than the 7 MeV usually employed. While the use of experimental splittings may be appropriate when calculations are made in a very limited basis, the exact values should be used when core excitations are included. The use of a lower value for the splitting will modify the results of shell-model calculations in the calcium region. For oxygen, the analogous $p_{1/2}$-$d_{5/2}$ splitting is only slightly overestimated when it is taken from binding energy data.

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[15] P. M. Endt and C. Van der Leun, Nucl. Phys. **A105**, 1 (1967).