be taken to ensure that the intrinsic determinant is of sufficient generality to include the correlations of importance. The quasiboson prescriptions for estimating ground-state densities, while simple, are unreliable unless the excitation energy is given correctly in the primary equations-of-motion calculation and unless only a few collective modes dominate the correlations. But if these conditions are satisfied, they appear to predict correlations of the correct magnitude. Further investigations by one of us[15] indicate, however, that for the ground-state correlations of vibrational nuclei, if a straightforward shell-model calculation is too difficult, then simple perturbation theory is probably the next best thing.

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Mixed-Parity Hartree-Fock Calculations for Light Nuclei Using Realistic Forces*

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Mixed-parity Hartree-Fock calculations have been performed on the nitrogen and oxygen isotopes using (1) a central Rosenfeld interaction, (2) a Rosenfeld-plus-an-appropriate-tensor interaction, and (3) bare Kuro-Brown matrix elements. It is shown that the results for the interactions (2) and (3) are fairly close. The gain for O^{16} is found to be larger than either of its isotopes $A=15$ or 17. This is interpreted in terms of the energy gap between the occupied and the unoccupied Hartree-Fock orbitals.

1. INTRODUCTION

THE parity mixing in the Hartree-Fock calculations was first indicated by Bleuler.[1] Since then a number of mixed-parity Hartree-Fock calculations have been reported in the literature.[2,3] The main purpose of such calculations is to see whether a better variational solution can be obtained by allowing parity mixing in the expansion of the single-nucleon orbitals. These mixed-parity solutions if they exist, are very useful in studying the configuration interaction problem when the mixings across the major harmonic-oscillator shells become important. This, for example, is the case for nuclei near closed shells, where particle-hole type of excitations are important.

Bassichis and Svenne[2] performed these calculations for the $4n$-type nuclei, using a model force derived from the Hamada-Johnston potential.[4] Their main conclusion was that it is sufficient to restrict the single-particle wave functions to be eigenfunctions of parity so long as the tensor part of the nuclear force is less than twice its accepted strength.

The mixed-parity Hartree-Fock calculations in Ref. 3 were carried out for the nitrogen and oxygen isotopes. A Rosenfeld central interaction was used in these calculations. These calculations had indicated that the mixed-parity single-particle orbitals can be obtained in the Hartree-Fock variational calculations provided the strength of the central potential is taken to be larger than the accepted value.

The purpose of the present calculation is to find the role played by the tensor force in the mixed-parity Hartree-Fock calculations for the light nuclei and then present the final results with realistic two-body matrix elements like the bare Kuo-Brown matrix elements,[5] which are derived from the Hamada-Johnston interaction.[4]

As in the earlier mixed-parity Hartree-Fock calculations,[3] we first discuss the two-level problem in Sec. 2, and then in Sec. 3 present the results for the expanded basis set with the bare Kuo-Brown matrix elements.

2. TWO-LEVEL HARTREE-FOCK CALCULATIONS

The two-level mixed-parity Hartree-Fock calculations are carried out by assuming the active nucleons move in the $1p_{1/2}$ and $1d_{5/2}$ orbitals outside of a $(1s_{1/2})^4(1p_{3/2})^8$ closed-shell core. The single-particle energies ϵ_{nlj} are taken from the experimental spectrum of the C^{13} nucleus and are given in Table I. These

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[1] K. Bleuler, in *Proceedings of the International School of Physics "Enrico Fermi"* (Academic Press Inc., New York, 1960), Course 36.
[2] W. H. Bassichis and J. P. Svenne, Phys. Rev. Letters **18**, 80 (1967).
[3] J. C. Parikh and Nazakat Ullah, Nucl. Phys. **A99**, 529 (1967).
[4] T. Hamada and I. D. Johnston, Nucl. Phys. **34**, 382 (1962).
[5] T. T. S. Kuo and G. E. Brown, Nucl. Phys. **85**, 40 (1966).

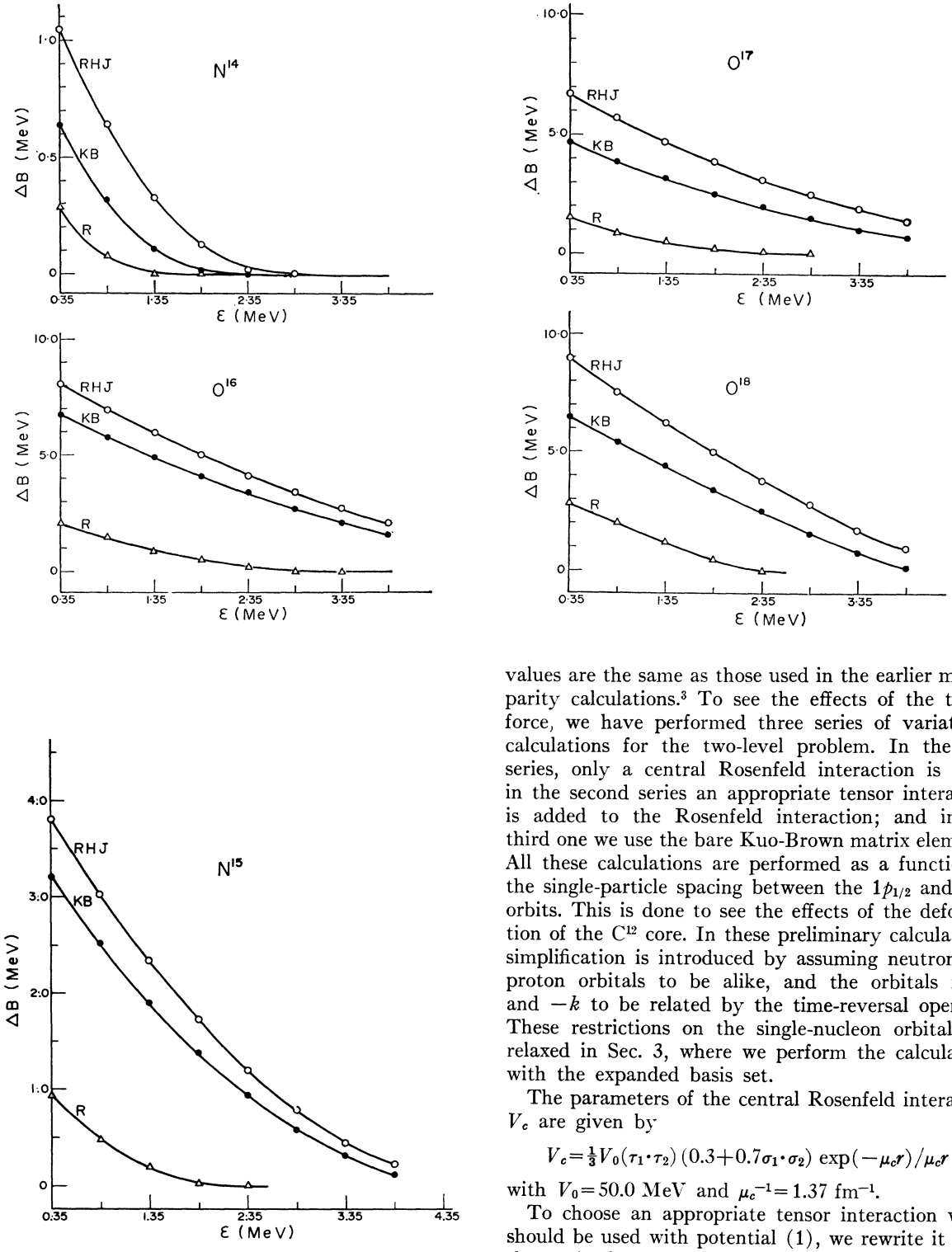

FIG. 1. Plot of the gain in binding energy ΔB against the single-particle spacing $\epsilon=\epsilon_{1d5/2}-\epsilon_{1p1/2}$ for the two-level problem. R, RHJ, and KB indicate Rosenfeld, Rosenfeld-plus-appropriate-tensor-component, and Kuo-Brown interaction, respectively.

values are the same as those used in the earlier mixed-parity calculations.[3] To see the effects of the tensor force, we have performed three series of variational calculations for the two-level problem. In the first series, only a central Rosenfeld interaction is used; in the second series an appropriate tensor interaction is added to the Rosenfeld interaction; and in the third one we use the bare Kuo-Brown matrix elements. All these calculations are performed as a function of the single-particle spacing between the $1p_{1/2}$ and $1d_{5/2}$ orbits. This is done to see the effects of the deformation of the C^{12} core. In these preliminary calculations, simplification is introduced by assuming neutron and proton orbitals to be alike, and the orbitals for k and $-k$ to be related by the time-reversal operator. These restrictions on the single-nucleon orbitals are relaxed in Sec. 3, where we perform the calculations with the expanded basis set.

The parameters of the central Rosenfeld interaction V_c are given by

$$V_c=\tfrac{1}{3}V_0(\tau_1\cdot\tau_2)\,(0.3+0.7\sigma_1\cdot\sigma_2)\,\exp(-\mu_c r)/\mu_c r \quad (1)$$

with $V_0=50.0$ MeV and $\mu_c^{-1}=1.37$ fm^{-1}.

To choose an appropriate tensor interaction which should be used with potential (1), we rewrite it using the projection operators in spin and isospin space

$$V_c=\tfrac{1}{3}V_0(P^{T=1,S=1}-1.8P^{T=1,S=0}-3.0P^{T=0,S=1}+5.4P^{T=0,S=0})\,\exp(-\mu_c r)/\mu_c r, \quad (2)$$

where $P^{T,S}$ is the projection operator, which projects out a wave function of definite isospin T and spin S from an arbitrary wave function. A comparison of the central and the tensor part of the Hamada-Johnston force tells us that the appropriate tensor force which should be used with interaction (2) is

$$V_T=\tfrac{1}{3}V_0(P^{T=1}-3P^{T=0})\{[3(\sigma_1\cdot r_{12})(\sigma_2\cdot r_{12})/r_{12}^2] -(\sigma_1\cdot\sigma_2)\}\exp(-\mu_T r)/\mu_T r \quad (3)$$

with $\mu_T^{-1}=1.415$ fm. In all our calculations the oscillator parameter b appearing in the radial wave function $-\exp[-\frac{1}{2}(r^2/b^2)]$ is taken to be 1.65 fm.

The results of the two-level calculation for the nitrogen and oxygen isotopes are shown in Fig. 1, where we have plotted the gain in binding energy ΔB due to parity mixing as a function of the single-particle spacing $\epsilon=\epsilon_{d_{5/2}}-\epsilon_{p_{1/2}}$ for the three interactions. The discussion of these results shall be taken up later in Sec. 4.

3. NUMERICAL CALCULATIONS USING EXPANDED BASIS SET

We now expand our basis set to include the $2s_{1/2}$ and $1d_{3/2}$ orbitals also. As we had mentioned earlier in Sec. 2, we shall carry out the mixed-parity Hartree-Fock calculations in the expanded basis set without assuming any time reversal invariance. Furthermore, the neutron and proton orbitals will be varied independently. The calculations are performed using the bare Kuo-Brown matrix elements[5] and the single-particle energies of Table I. In Table II we show the gain in binding energy due to parity mixing in the expanded basis set. Table III gives the eigenvalues and the eigenvector components of the mixed-parity single-particle Hartree-Fock operator.

4. DISCUSSIONS OF RESULTS

The following observations are made by looking at the plots of gain in binding energy against the single-particle spacing shown in Fig. 1: (a) For purely central forces the gain in binding energy is zero for all the nitrogen and oxygen isotopes unless the single-particle spacing is very small. This is the same result which we had found earlier[3]; it is used as a check on the present calculations. The fact that parity mixing is very small if one uses purely central forces is also in agreement with the arguments of Banerjee, Levinson, and Stephenson.[6] (b) The tensor component in the two-body force increases the gain in binding energy. The results obtained with the bare Kuo-Brown matrix elements are fairly close to the ones given by the force which is a combination of the central Rosenfeld interaction and an appropriate tensor force. We therefore conclude that the effects of a noncentral tensor force can be reproduced if one adds the tensor component given by expression (3) to the usual Rosenfeld force. (c) The gain in binding energy is small for normal single-particle spacing. It is maximum for O^{16} and is less for either of the isotopes $A=15$ or 17. This feature remains true even when the basis set is expanded (Table II).

TABLE I. Single-particle energies ϵ_{nlj}.

State nlj	Energy ϵ_{nlj} (MeV)
$1p_{1/2}$	−4.95
$2s_{1/2}$	−1.86
$1d_{5/2}$	−1.10
$1d_{3/2}$	3.39

TABLE II. Gain in binding energy ΔB due to parity mixing.

Nucleus	Gain in binding energy ΔB (MeV)
N^{14}	0.0
N^{15}	0.573
O^{16}	1.677
O^{17}	0.798
O^{18}	0.255

The results of Table III are obtained without assuming any time reversal invariance or the equivalence of neutron and proton wave functions. We see from this table that for a doubly closed nucleus like O^{16}, the final solutions do converge to the ones which have time reversal invariance and neutron and proton wave functions alike. These symmetries are destroyed for the open-shell nuclei like N^{15}. Since no Coulomb force is included in the Hamiltonian, and the single-particle energies ϵ_{nlj} are taken to be the same for neutron and proton, the Hartree-Fock (HF) orbitals for O^{15} are obtained from those of N^{15} by interchanging neutron and proton.

It should be pointed out that there is no spurious state problem due to center-of-mass motion in our solution for the two-level case. In the expanded basis, spurious states can enter into the solution, but since the trend is identical to that of the two-level case, we believe the admixture is small.

Perhaps the most interesting result of our calculation is that the gain in binding energy for O^{16} is more than any of its isotopes $A=15$ or 17. This is true for all three interactions which we have used and also for the expanded basis set. To explain this, let us suppose that we have performed two HF calculations, one spherical with js being a good quantum number, and the other deformed with only k being a good

[6] M. K. Banerjee, C. A. Levinson, and G. J. Stephenson, Phys. Rev. 178, 1709 (1969).

TABLE III. Eigenvalues $\epsilon_{km\tau}^{\mathrm{HF}}$ and the eigenvector components $C_{nlj}^{km\tau}$ of the HF single-particle Hamiltonian for the nitrogen and oxygen isotopes.

Nucleus	$\phi_{km\tau}$		$\epsilon_{km\tau}^{\mathrm{HF}}$	$1p_{1/2}$	$2s_{1/2}$	$1d_{5/2}$	$1d_{3/2}$
N^{14}	$\frac{1}{2}$	$\frac{1}{2}$	−7.534	1.000	0.000	0.000	0.000
	$\frac{1}{2}$	$-\frac{1}{2}$	−7.534	1.000	0.000	0.000	0.000
N^{15}	$\frac{1}{2}$	$-\frac{1}{2}$	−9.659	0.948	0.014	−0.314	0.052
	$\frac{1}{2}$	$\frac{1}{2}$	−9.389	0.880	−0.012	0.474	−0.022
	$-\frac{1}{2}$	$\frac{1}{2}$	−7.855	0.892	−0.003	0.451	0.040
O^{16}	$-\frac{1}{2}$	$-\frac{1}{2}$	−11.209	0.866	0.031	−0.494	0.068
	$-\frac{1}{2}$	$\frac{1}{2}$	−11.209	0.867	0.032	−0.493	0.068
	$\frac{1}{2}$	$\frac{1}{2}$	−11.138	0.868	−0.025	0.497	−0.007
	$\frac{1}{2}$	$-\frac{1}{2}$	−11.137	0.868	−0.025	−0.496	−0.007
O^{17}	$-\frac{1}{2}$	$-\frac{1}{2}$	−13.301	0.925	−0.007	−0.373	0.073
	$\frac{1}{2}$	$-\frac{1}{2}$	−13.092	0.922	0.028	0.385	−0.002
	$\frac{1}{2}$	$\frac{1}{2}$	−12.208	0.916	−0.006	0.400	0.025
	$-\frac{1}{2}$	$\frac{1}{2}$	−12.463	0.884	−0.011	−0.466	0.044
	$\frac{5}{2}$	$\frac{1}{2}$	−8.170	0.000	0.000	1.000	0.000
O^{18}	$-\frac{1}{2}$	$-\frac{1}{2}$	−15.352	0.961	−0.035	−0.267	0.061
	$\frac{1}{2}$	$-\frac{1}{2}$	−15.279	0.963	0.035	0.266	−0.005
	$\frac{1}{2}$	$\frac{1}{2}$	−12.493	0.939	0.020	0.341	0.037
	$-\frac{1}{2}$	$\frac{1}{2}$	−12.490	0.940	−0.012	−0.341	0.018
	$-\frac{5}{2}$	$\frac{1}{2}$	−9.596	0.000	0.000	1.000	0.000
	$\frac{5}{2}$	$\frac{1}{2}$	−9.589	0.000	0.000	1.000	0.000

quantum number. The gain in binding energy for the O^{16} nucleus is defined by

$$\Delta B(O^{16}) = E(p_{1/2})^4 - E(|k| = \tfrac{1}{2})^4, \quad (4)$$

where $E(p_{1/2})^4$ is the energy of the four nucleons in the $p_{1/2}$ orbit, and $E(|k| = \frac{1}{2})^4$ is the energy when four nucleons occupy $\phi_{k=\pm 1/2}$ orbits. From the Hartree-Fock calculation of O^{16}, we can construct the wave functions for O^{15} and O^{17} by destroying and creating a neutron, respectively, and calculating the corresponding ΔB for these two nuclei. It is easy to show that

$$\Delta B(O^{17}) = \Delta B(O^{16}) - [\langle \phi_{k=(5/2)n} | h^{\mathrm{def}} | \phi_{k=(5/2)n} \rangle - \langle d_{(5/2)n} | h^{\mathrm{sph}} | d_{(5/2)n} \rangle], \quad (5a)$$

$$\Delta B(O^{15}) = \Delta B(O^{16}) - [\langle p_{(1/2n)} | h^{\mathrm{sph}} | p_{1/2n} \rangle - \langle \phi_{k=(1/2n)} | h^{\mathrm{def}} | \phi_{k=(1/2n)} \rangle], \quad (5b)$$

where h^{sph} and h^{def} are the single-particle spherical and deformed HF Hamiltonians for the O^{16} nucleus. We see from expressions (5a) and (5b) that the gains $\Delta B(O^{15})$ and $\Delta B(O^{17})$ will be smaller than $\Delta B(O^{16})$ if the single-particle levels $k=\frac{1}{2}n$ and $k=\frac{5}{2}n$ in the deformed HF calculation are pushed down and up, respectively, relative to the spherical $p_{1/2}$ and $d_{5/2}$ levels. We have calculated these quantities from our HF calculations and find that the above behavior of the energy gap for the spherical and deformed Hartree-Fock is true.

We therefore see that the gain in binding energy in the mixed-parity calculations is closely related to the energy gap between the occupied and the unoccupied HF orbitals. It will be interesting to see whether the above type of behavior is also observed for isotopes of other $4n$-type nuclei.

We remark here that Bar-Touv and Levinson,[7] and also recently Rowe,[8] in their HF calculations on light nuclei have observed that a single-particle HF level starts sinking from its unoccupied position to its fully occupied position as it becomes occupied, while the other levels remain relatively unshifted. Let us now consider the positions of the $p_{1/2}$ and $d_{5/2}$ levels in the isotopes of O^{16} using this picture. The $p_{1/2}$ level gets fully occupied at O^{16} and this should be its lowest position, while the position of the $d_{5/2}$ level both in $A=15$ and 16 should almost be the same. When we go to $A=17$, then the $d_{5/2}$ level starts getting filled and therefore it should sink relative to the one in O^{16}, while the $p_{1/2}$ levels both in $A=16$ and 17 should almost remain unshifted. This means that the gap will be bigger for $A=16$ than either of the nuclei $A=15$ or 17. This, combined with the results of Fig. 1, tells us that the gain in binding energy due to parity mixing is bigger for the nucleus which has a bigger gap.

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[7] J. Bar-Touv and C. A. Levinson, Phys. Rev. **153**, 1099 (1967).
[8] D. J. Rowe (private communication).