State Dependence of Coulomb Interaction in Nuclei*

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The Coulomb energies of valence particles in Ne^{18} and Ti^{42} are calculated using realistic two-particle wave functions. The extra correlation in the configuration-mixed wave functions increases the Coulomb interaction by ~150 keV for the 0^+ state, and ~50 keV for the 2^+. This large effect brings the theoretical binding-energy differences of the mass-18 and mass-42 isospin triplets into agreement with experiment, but yields an average interaction larger than required by the binding-energy systematics of heavier nuclei.

I. INTRODUCTION

BECAUSE the Coulomb force is long range, the Coulomb interaction between particles in the nucleus depends mostly on the average size of the single-particle wave functions. It has long been known that there is some state dependence to the interaction, but it has never been calculated very accurately. Feenberg and Goertzel[1] first considered the effect arising from the symmetry of the wave function: Space symmetric protons are closer together on the average and so have a larger than average Coulomb interaction. This produces a visible effect on the systematics of Coulomb energies of mirror nuclei, as discussed by Carlson and Talmi.[2] These authors calculated the effect with j-j coupled wave functions and assumed pairing wave functions for the nuclei. The orders of magnitude found for the $d_{5/2}$ shell were 0.41-MeV average interaction and 0.15-MeV pairing, somewhat larger than calculated.[3]

We will calculate the Coulomb interaction in a two-particle wave function allowing configuration mixing. We know that the correlations induced by configuration mixing are needed for a quantitative explanation of some nuclear properties, such as the binding of 0^+ states or the two-particle transfer cross sections. It should not be surprising that the same correlations have a substantial effect on the Coulomb energy.

II. CALCULATION

We calculate the Coulomb interaction of the last two protons in Ne^{18} and Ti^{42}. The single-particle wave functions were taken to be harmonic-oscillator functions of the standard parameters $\nu=0.35$ and $\nu=0.27$, where $\psi\sim\exp(-\nu r^2/2)$. Using the more realistic Woods-Saxon well wave functions would not substantially change the results, because the two functions differ only in the tail region where there is a small probability amplitude anyway. The configuration mixture amplitudes were taken from Kuo,[4] who derived the wave functions from a realistic two-body interaction and obtained impressive agreement with experiment on the two-particle spectra.[5]

For orientation on the size of correlation effect to expect we quote Kuo's wave function for the $J=0$ $T=1$ ground state of Ca^{42}, Sc^{42}, and Ti^{42}:

$$\psi(0^+)=0.927|(f_{7/2}f_{7/2})^0\rangle+0.203|(p_{3/2}p_{3/2})^0\rangle +0.203|(f_{5/2}f_{5/2})^0\rangle+0.109|(p_{1/2}p_{1/2})^0\rangle -0.217|(g_{9/2}g_{9/2})^0\rangle. \quad (1)$$

Each of these components has an amplitude roughly proportional to $(-1)^l(2j+1)^{1/2}$ for the two particles being together at the nuclear surface. Adding amplitudes gives a total probability enhancement of 19 for the correlation, as compared with 8 for pure $(f_{7/2}f_{7/2})^0$ and 1 for uncorrelated particles. Thus for strictly short-range effects we would expect a doubling of matrix elements in the correlated 0^+. The Coulomb force, proportional to $1/r$, is much smoother but can still be substantially enhanced by the correlations.

To evaluate the expectation of the Coulomb interaction we use the expression

$$E_{\mathrm{Coul}}{}^J=e^2\sum_{\substack{\text{all } j,l,n\\ \mathfrak{L},L,S}} a_{jj'}{}^J a_{j''j'''}{}^J(jj'|l_1l_2\mathfrak{L}S)_J \times(j''j'''|l_3l_4\mathfrak{L}S)_J(n_1l_1n_2l_2|nlNL)_{\mathfrak{L}} \times(n_3l_3n_4l_4|n'l'NL)_{\mathfrak{L}}\langle nl|1/r|n'l'\rangle. \quad (2)$$

Here $a_{jj'}{}^J$ are the configuration admixture amplitudes of the state $(jj')^J$ in the eigenstate. The recoupling coefficients are the usual LS-jj coefficients and Moshinsky's brackets to transform from single-particle wave functions to center-of-mass and relative coordinate wave functions.[6] The matrix element of $1/r_{12}$ in relative coordinates requires a simple one-dimensional integral.[7]

The states included by Kuo for the $f_{7/2}$ calculation are the fp shell and $g_{9/2}$. Although the intermediate energy for the $g_{9/2}g_{9/2}$ configuration is high, there is a strong matrix element of the potential connecting this state. It turned out that the $g_{9/2}$ has an important

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[1] E. Feenberg and G. Goertzel, Phys. Rev. **70**, 597 (1946).
[2] B. C. Carlson and I. Talmi, Phys. Rev. **96**, 436 (1954).
[3] A. de-Shalit and I. Talmi, *Nuclear Shell Theory* (Academic Press Inc., New York, 1963), p. 347.
[4] T. T. S. Kuo and G. E. Brown, Nucl. Phys. **A114**, 241 (1968).
[5] T. T. S. Kuo and G. E. Brown, Nucl. Phys. **85**, 40 (1966).
[6] T. A. Brody and M. Moshinsky, *Tables of Transformation Brackets* (University of Mexico, 1960).
[7] The author thanks L. Zamick for a numerical table of the matrix elements of $1/r$.

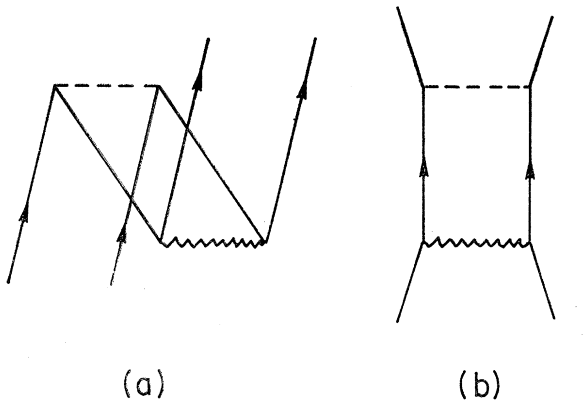

FIG. 1. Perturbation graphs included in calculation of Coulomb energy. (a) is a ground-state correlation graph involving a 4-particle 2-hole intermediate state. One interaction is nuclear and the other is Coulomb. (b) is a 2-particle correlation, and is included either to this order in perturbation theory or to all orders when a matrix is diagonalized. Both graphs have the same over-all sign.

influence on the Coulomb interaction because it breaks the single-particle parity. Otherwise, no matter how strong the correlation is, there would be an equally strong anticorrelation. Other levels in the g shell with radial nodes do not contribute significantly.

In perturbation theory, the ground-state correlation graph, Fig. 1(a), contributes to the same extent as the $2\hbar\omega$ excitation of Fig. 1(b). The latter is represented by the $g_{9/2}g_{9/2}$ configuration and is already included. We therefore included ground-state correlations in second-order perturbation theory, even though the entire enhancement of the Coulomb interaction can no longer be interpreted as a simple two-particle correlation. Numerically, this graph produces an effect of the order of 50 keV in the 0^+ state and a negligible effect in higher-J states.

For the $d_{5/2}$ calculation, Kuo's wave function[5] has explicit components only for the sd shell, so both Figs. 1(a) and 1(b) were calculated as perturbations. The off-diagonal matrix elements involved were calculated by Kuo,[8] and the energy denominators were taken as 25 MeV for Ne^{18} and 19 MeV for Ti^{42}. The results, shown in Table I, show an enhancement of the Coulomb energy in all states, with a dramatic effect in the 0^+, of about 150 keV.

III. COMPARISON WITH EXPERIMENT

Experimentally, two types of interaction energies are measured. The first is the interaction in the two-particle states of definite J, obtained from the binding energies of the $T=1$ triplet by

$$V_{\text{Coul}}=E(T_z=1)+E(T_z=-1)-2E(T_z=0). \quad (3)$$

For the 0^+, this is the ground state of the mass-42 system and the binding energies are quite well determined

[8] T. T. S. Kuo (private communication).

TABLE II. Coulomb interaction (keV) between valence protons. The experimental average interaction is from systematics of nuclei filling the shell. The experimental interaction in states of different J is from the binding energies of the 2-particle nuclei. The row "uncorrelated" shows the calculated energy for pure j-j coupled wave functions, and the row "correlated" uses the realistic wave function. For the calculation, the average was taken as the $(2J+1)$-weighed average over all J.

	Average interaction	$J=0$	$J=2$	$J=4$	$J=6$
	Ne^{18} $\nu=0.35$				
Experimental	412	701	510	405	
Reference	[a]	[b,c,d]			
Uncorrelated	412	490	424	394	
Correlated	459	634	496	419	
	Ti^{42} $\nu=0.27$				
Experimental	300	550	450	?	?
Reference	[e]	[f,g]			
Uncorrelated	320	406	346	316	308
Correlated	340	550	407	338	316

[a] Reference 3.
[b] J. H. E. Mattauch, W. Thiele, and A. H. Wapstra, Nucl. Phys. 67, 1 (1964).
[c] Reference 9.
[d] S. Gorodetzky *et al.*, Phys. Rev. 155, 1119 (1967).
[e] R. Sherr, Phys. Letters 24B, 321 (1967).
[f] J. J. Schwartz *et al.*, Phys. Rev. Letters 19, 1482 (1967).
[g] M. Shapiro (private communication).

with recent data.[9] This is also true for the mass-18 triplet where the F^{18} state is an excited state. As seen in Table I, the Coulomb interaction is very large, nearly comparable to that in the He^3–T system.

For states of other J, we need the spectra of the $T=1$ triplet, and then use Eq. (3) with the binding energies of the excited states. The experimental situation is shown in Fig. 2. In the mass-18 system the only doubtful state is the 4^+ in Ne^{18}, which was taken as the 3.362-MeV state.[10] The situation is worse in the mass-42 system, where the 4^+ and 6^+ are uncertain in both Sc^{42} and Ti^{42}.

One point of concern in the analysis is that the spectra of the nn and the np nuclei are not identical. This could be caused by admixtures of many-particle many-hole states, or indeed by anything else that changes the single-particle occupation probabilities of the states. Fortunately, most of these effects, except for the one in Fig. 1(a), seem to be linear in the number of protons and therefore would not affect the Coulomb interaction as calculated by Eq. (3).

The agreement between calculation and experimental binding energies is good, as may be seen by Fig. 3. There is no doubt that configuration mixing is present in these nuclei, and is needed to explain the Coulomb shifts quantitatively.

A second kind of experimental evidence is the systematics of binding of many nuclei in the shell. The average interaction is calculated by averaging over the interaction in states of definite J with a $(2J+1)$ weighing factor. The experimental average interaction is in clear disagreement with the calculation. Protons do not seem to be as well correlated in many-particle nuclei as in the two-particle nuclei. A different weighing

[9] R. G. Miller and R. W. Kavanagh, Nucl. Phys. A94, 261 (1967).
[10] E. Adelberger (private communication).

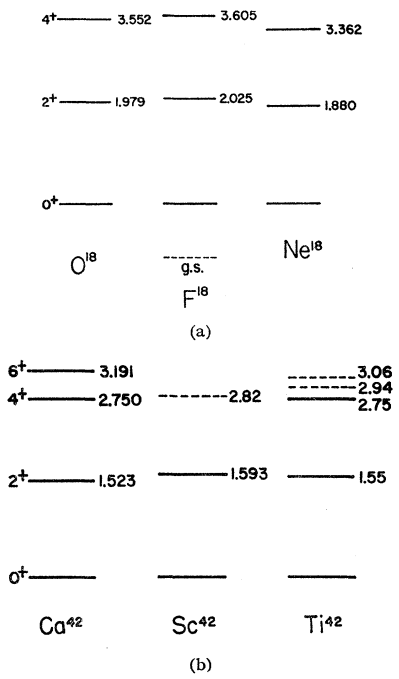

FIG. 2. Spectra of $T=1$ triplets of mass 18 and 42. References are: O^{18} [*Nuclear Data Sheets*, edited by K. Way *et al.* (National Academy of Sciences–National Research Council, Washington 25, D. C. (1966)]; F^{18} [S. Gorodetzky *et al.*, Phys. Rev. **155**, 1119 (1967)]; Ne^{18} (Ref. 10); Ca^{42} [J. W. Nelson *et al.*, Nucl. Phys. **62**, 434 (1965)]; Sc^{42} [J. J. Schwartz *et al.*, Phys. Rev. Letters **19**, 1482 (1967)]; Ti^{42} [Ref. 8; and M. Shapiro (private communication)]. A large state dependence is visible in the mass-18 spectra, where the 4^+ state is shifted relative to the others.

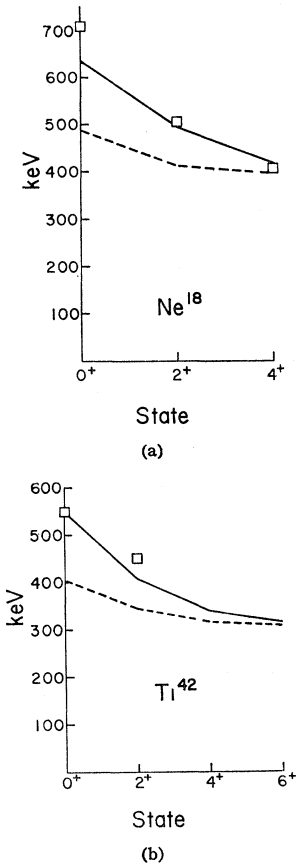

FIG. 3. Comparison of theoretical and experimental Coulomb interactions in 2-particle states from Table I. Squares are experimental, solid lines calculation with correlated wave functions, and broken lines calculation with pure j-coupled wave functions.

could be used in the average, depending on the many-body wave function assumed, but this would probably emphasize $J=0$ and make matters worse.

In view of the success with the two-particle nuclei, we do not understand the disagreement in the more complicated nuclei. It might be thought that Graph 1(a) would be cut down by the exclusion principle when the proton shell is filled, but this would not affect the average energy significantly. The two-particle correlation itself should involve states of high enough energy so that it would not be affected by details of the neutron configurations. It is only if the neutrons produce a substantial change in the $f_{7/2}$ occupation by the protons that we would expect a change in the average interaction. This might happen, for example, if the neutrons induced a transition to a deformed state. If this is the case it has not yet been observed by particle reactions.

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