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Comparison of Realistic and Empirically Optimized Nuclear Hamiltonians*

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Empirically determined Hamiltonians for A=18-24 and A=32-38 nuclei exhibit average attractions between unlike active orbits which are only half as strong as those obtained when corresponding effective Hamiltonians are calculated from nucleon-nucleon parameters and corrected for core-polarization effects.

The calculation of an effective nuclear Hamiltonian from the parameters of the nucleon-nucleon system is a fundamental project of nuclear structure theory. Major problems in successfully executing this project involve treatment of the hard core of the nucleon-nucleon interaction and of the effects of truncation to a finite-basis model space. Extensive effort has been devoted both to carrying through such calculations[1-4] to obtain "realistic" model interactions and to investigating the validity of the approximations employed.[5-7] Despite the many apparently successful applications to shell model[8-10] and Hartree-Fock[11,12] calculations of these realistic interactions, exemplified by those of Kuo and Brown,[1] there remains considerable uncertainty not only as to the details of the correct effective Hamiltonian but also as to the soundness of some of the basic steps in the theory used to obtain them.

We have obtained[13] empirical adjustments to the matrix elements of realistic interactions for the sd-shell such that the resulting Hamiltonians yield the best possible simultaneous agreement with the level energies in nuclei of several consecutive mass numbers. In this note we describe the qualitatively significant changes in the realistic Hamiltonians which the energy level data from multiparticle systems demand, and some consequences of these changes. We also discuss the extent to which these multiparticle spectra require state and mass dependence in the model Hamiltonians.

We consider Hamiltonians for the lower and upper halves of the sd-shell. The Hamiltonian for A=18-28 was determined by iteratively adjusting Kuo's $\hbar\omega$=14 MeV two-body matrix elements[2,8] so as to obtain a converged minimum rms fit of shell-model eigenvalues (diagonizations carried out in the full $d_{5/2}$-$s_{1/2}$-$d_{3/2}$ basis space) to almost 200 experimental nuclear binding energies. The data were taken in the main from the A=18-24 region. The Hamiltonian for A=28-38 was obtained by similarly adjusting Kuo's $\hbar\omega$=12.5 MeV interaction[2,9] to fit 140 level energies taken from A=32-38 nuclei. The single-particle energies associated with the two interactions are chosen to reproduce, respectively, the ^{17}O and ^{39}K spectra of single-particle states. Calculations with these two Hamiltonians show that spectra of A=18-26 nuclei are reproduced to an rms deviation per level of <250 keV and spectra of A=32-38 nuclei to an rms of <300 keV.

The elements of the technique utilized in determining the present empirical interactions are described in an appendix to ref. 8. A key improvement incorporated into the present work involves use of the eigenvectors of the error matrix of the fit equations to transform the two-body matrix elements into a set of

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Hamiltonian parameters which are mutually linearly independent with respect to the data base. The eigenvalues of these transformation vectors are a measure of how well the data set determines the various combinations of two-body matrix elements. In addition to overcoming some of the problems associated with correlations between two-body matrix elements, use of these transformed parameters thus permits the adjustment of the better determined parameters while the poorer determined combinations are held fixed to the starting values. Plots of the eigenvalues of the inverse error matrix (see Figure 1) show that surprisingly few of the 63 two-body parameters have greater than a ~1% effect on the experimental-theoretical rms deviation.

Calculations of realistic interactions are typically made only for two-body systems, and there are many theoretically plausible sources for strong state- and mass-dependent renormalizations of the Hamiltonians for many-body systems. Hence is important to consider whether the changes we make in the realistic values can be meaningfully considered improvements or whether they result from the procrustean forcing of a constant-valued Hamiltonian onto a data set demanding a more complex formulation. A definitive answer is unavailable. However, the quality of the fits to energy levels obtained over the present mass ranges of 8 particles is comparable to results from similar fits to over ranges of only 6 and 4 particles,[14,8] and it can be argued that the size of the deviations are appropriate in the larger context of the application of the shell-model to these nuclei. Also, essential features of our results are consistent with the results of an analysis[15] of the particle-transfer strengths of the two-body system ^{18}O.

The key features which result from the empirical adjustments to the two realistic Hamiltonians are summarized in Table I. The members of a given family (j_1j_2) of diagonal two-body matrix elements are weighted by the spin and isospin statistical factors and summed to yield values of the average two-body attraction between nucleons in orbits j_1 and j_2. It is striking that the well-determined final empirical values for like orbits ($j_1=j_2$) are very similar to the original realistic values. Even more striking, however, is the consistent factor of ~2 reduction from the realistic to the empirical values which is found for the strength of the attraction between unlike orbits ($j_1 \neq j_2$). The stability of this effect and its large size argue convincingly that the currently used realistic interactions produce significantly too much attraction between particles in different shell-model orbits. These conclusions are consistent with those of earlier, less systematic studies.[14,16]

For systems of a few (≤ 5) active particles (or holes) the effects of this over-attractiveness are not strongly manifested in shell-model calculations[8,9] because the one-body energies dominate the structure of the multiparticle spectra. However, advances in computational techniques have recently made possible shell-model calculations for up to 12 active particles in the full sd-shell basis. Such calculations made with realistic interactions have shown severe pathologies, such as large overbinding and incorrect ground-state spins.[17,18] For larger numbers of active particles, the two-body part of the Hamiltonian almost completely swamps the influence of the single-particle spectrum and it is vital to have the best possible (in the empirical sense) set of two-body matrix elements. The present interactions succeed in yielding uniform reproductions of binding and excitation energies at the ≃250 keV deviation level up through 9 particles or holes. Spectra continue to be well-reproduced on through the 12-particle systems although >2 MeV total-binding-energy deviations have built up by ^{28}Si. Beyond 12 particles or holes the calculated energies clearly show the need for changes in the Hamiltonians.

Our empirical adjustments to the realistic Hamiltonians have profound consequences for wave functions of many-particle systems. Shown in Figure 2 are characteristics of the ^{28}Si ground state wave functions obtained in calculations with the two empirical Hamiltonians and the $\hbar\omega$=14 MeV interaction of Kuo. The plot of intensity versus the occupation of $d_{5/2}{}^n$ configurations graphically shows the degree of sub-shell closure at N=12 obtained with the various interactions. It is seen that the almost statistical distribution of configuration strength, which is apparently[19] a general feature of realistic Hamiltonians, is in no sense a "shell-model" result but rather a result of a particular type of Hamiltonian. Hamiltonians which best reproduce the spectra of either lighter or heavier multiparticle sd-shell nuclei predict a quite different result, one with a skew towards $d_{5/2}$ closure at ^{28}Si.

In conclusion, we first emphasize that it appears that there is good reason to suspect that previous calculations of realistic effective interactions yield about twice too much attraction between unlike shell-model orbits. It should be very worthwhile to attempt to isolate the origin of this result. Second, we note that the empirically best Hamiltonians for the sd-shell are so different from the realistic interactions that use of the realistic values for many (>6) particle systems should not be expected to give quantitative reproduction of the features of actual nuclei.

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TABLE I.--Strengths ($\sum_{J,T}(2J+1)(2T+1)\langle j_a j_b|V|j_a j_b\rangle_{JT}$) in MeV of orbit-orbit interactions of realistic and empirical effective interactions. The empirical values marked with asterisks were not well determined in the fitting processes because the preponderance of levels in the respective regions do not involve those orbits.

j_a	j_b	$\hbar\omega$=14 MeV[a]	A=18-24	$\hbar\omega$=12.5 MeV[b]	A=32-38
5/2	5/2	- 73.6	-77.4	- 62.5	-42.5*
5/2	1/2	- 44.6	-20.5	- 37.6	- 7.9*
5/2	3/2	-133.1	-74.5	-115.0	-56.6
1/2	1/2	- 15.4	-16.9	- 14.2	-12.5
1/2	3/2	- 20.8	-16.0*	- 18.1	-10.0
3/2	3/2	- 20.8	-19.5*	- 18.3	-18.5

[a] Reference 2.

[b] Reference 2,9.

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FIGURE CAPTIONS

Fig. 1.--Illustration of the decreasing influence of a 200 keV change in the successively less-well-determined linearly independent ("orthogonal") combinations of two-body matrix elements upon the rms (labeled χ^2) deviation between shell-model eigenvalues and experimental energies. The solid points result from the A=18-24 fit, the open points from the A=32-38 fit.

Fig. 2.--Illustration of the percentage of the ^{28}Si ground-state wave function which is apportioned to each configuration $(d_{5/2})^n\ (s_{1/2}-d_{3/2})^{12-n}$ as calculated with the A=18-24 ("particle") and A=32-38("hole) empirical Hamiltonians and the Kuo (ref. 2) $\hbar\omega$=14 MeV Hamiltonian.

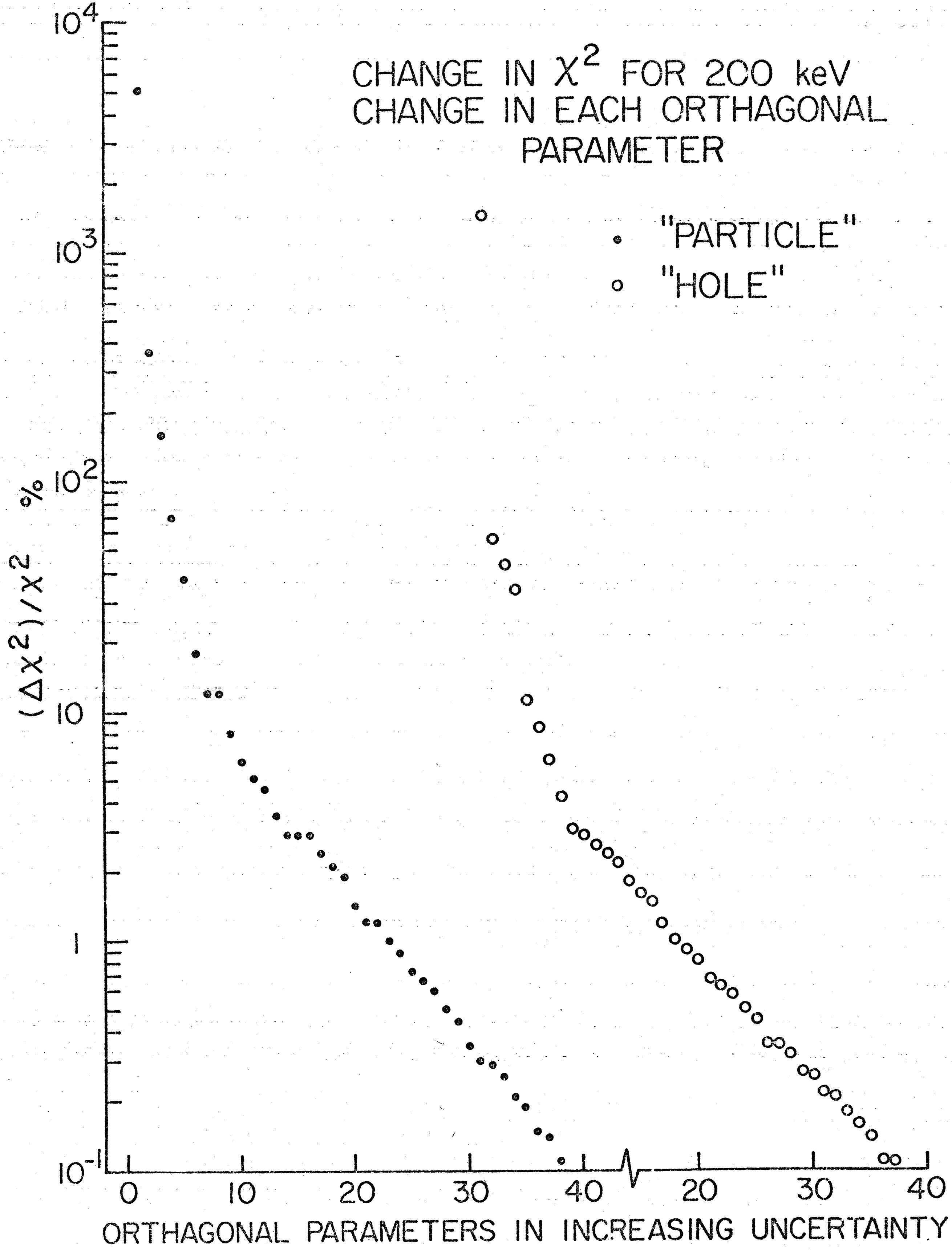
CHANGE IN χ^2 FOR 200 keV
CHANGE IN EACH ORTHAGONAL
PARAMETER
"PARTICLE"
"HOLE"
$(\Delta\chi^2)/\chi^2$ %
10^4
10^3
10^2
10
1
10^{-1}
0
10
20
30
40
20
30
40
ORTHAGONAL PARAMETERS IN INCREASING UNCERTAINTY

Figure 1

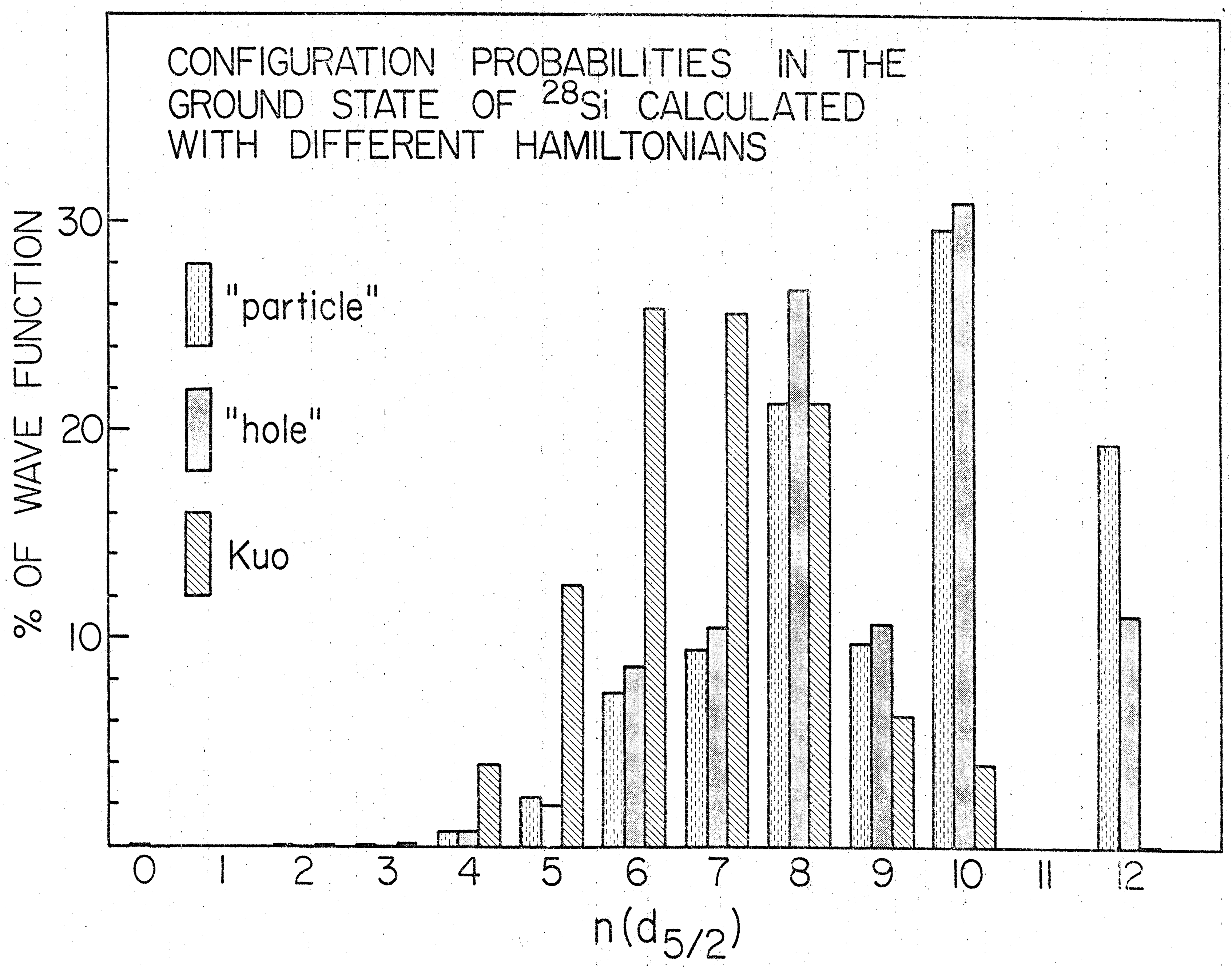

Figure 2

CONFIGURATION PROBABILITIES IN THE GROUND STATE OF ^{28}Si CALCULATED WITH DIFFERENT HAMILTONIANS