Influence of Saturation Properties on Shell-Model Calculations

A. Abzouzi, E. Caurier, and A. P. Zuker
Centre de Recherches Nucléaires, Institut National de Physique Nucléaire et de Physique des Particules, Université Louis Pasteur, B.P. 20, 67037 Strasbourg CEDEX, France
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It is shown that the nuclear Hamiltonian $\mathcal{H}$ separates rigorously into a monopole field $\mathcal{H}_m$ and a multipole part $\mathcal{H}_M$. $\mathcal{H}_m$ is entirely responsible for saturation properties and can be treated phenomenologically with few parameters. When realistic interactions are used for $\mathcal{H}_M$ in regions from the p shell to the $N=82$ isotones, shell-model calculations yield excellent spectroscopy and demand nuclear radii very close to the observed ones.

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The use of realistic potentials (i.e., consistent with NN scattering) in shell-model calculations was pioneered by Kuo and Brown[1] (KB). Of the enormous body of work that followed we would like to extract two basic observations.

The first is that whatever the forces (hard or soft core, ancient or new) and the method of regularization (Brueckner G matrix,[1,2] Sussex direct extraction,[3] or Jastrow correlations[4]), the effective matrix elements are *extraordinarily similar*.[5,6] The most recent results[7] amount to a vindication of the original work of Kuo and Brown. We take this similarity to be the great strength of realistic interactions, since it confers on them a model-independent status as direct links to the phase shifts.

The second observation is that when used in shell-model calculations and compared with data these matrix elements lead to results that deteriorate rapidly as the number of particles increases.[8,9] It was found[5] that in the fp region a phenomenological cure, confirmed by exact diagonalizations[10] up to $A=48$, amounts to very simple modifications of the centroids of the KB interaction.[11] It may be obvious, but we shall demonstrate it explicitly, that the need for such a cure reflects the failure of nonrelativistic potentials to saturate properly.[12,13]

Saturation properties dictate the equilibrium radius and energy of nuclei through some form of Hartree-Fock (HF) self-consistency. Our program consists in showing that once these properties are correctly enforced phenomenologically, the realistic interactions give a very sound description of correlations and detailed structure. We proceed in three steps.

(I) The nuclear Hamiltonian is shown to separate rigorously in two terms $\mathcal{H}=\mathcal{H}_m+\mathcal{H}_M$. The monopole field $\mathcal{H}_m$ is entirely responsible for spherical HF self-consistency and its generalization to open shells. The multipole part $\mathcal{H}_M$ acts as residual interaction.

(II m) Good saturation properties in $\mathcal{H}_m$ are enforced by introducing directly as parameters observed closed-shell and single-particle energies.

(II M) The nuclear radii at which $\mathcal{H}_M$ is calculated are allowed to vary freely and adopt values consistently close to the observed ones.

(III) Shell-model calculations in the p and sd regions and for the $N=50,82$ isotones and $Z=28,50$ isotopes then establish the soundness of the realistic $\mathcal{H}_M$. Our choice of the Kahana, Lee, and Scott (KLS) interaction[2] is made owing to availability[14] but rests on the observation in the second paragraph above.

(I) Separation properties.—A properly regularized potential is density dependent, nonlocal, and of a rank higher than 2. However, since these complications are mostly related to saturation, which we shall treat phenomenologically, we assume that our Hamiltonian is a sum of kinetic (K) and two-body terms (V), and we perform on it a preliminary separation $\mathcal{H}=\mathcal{H}_m^d+\mathcal{H}_M^d$ (d for diagonal),

$$\mathcal{H}_m^d=\sum K_{rr}n_r+\sum_{r\le s}\left[V_{rs}n_{rs}+b_{rs}\left(T_r\cdot T_s-\frac{3n_r\bar{n}_s}{4(N_r-1)}\delta_{rs}\right)(1+\delta_{rs})^{-1}\right]. \tag{1}$$

Here n_r and T_r are the number and isospin operators for shell r which has degeneracy $N_r=2(2j_r+1)$. Also, $\bar{n}_r=N_r-n_r$, $n_{rs}=n_r(n_s-\delta_{rs})(1+\delta_{rs})^{-1}$ (same notation for N_{rs}). K_{rr} and V^{JT}_{rstu} are the one- and two-body matrix elements,

$$V_{rs}=\sum V^{JT}_{rsrs}(2J+1)(2T+1)\Big/\sum(2J+1)(2T+1)\,,\quad b_{rs}=V^1_{rs}-V^0_{rs},\quad V^T_{rs}=\sum V^{JT}_{rsrs}(2J+1)\Big/\sum(2J+1)$$

(sums over Pauli-allowed values of J,T). $\mathcal{H}_M^d$ is the two-body part of the interaction with V^{JT}_{rstu} replaced by $W^{JT}_{rstu}=V^{JT}_{rstu}-V^T_{rs}\delta_{rt}\delta_{su}$.

The important property of $\mathcal{H}_m^d$ is that it reproduces the average energy of a configuration at fixed n_r,T_r for each

shell.[15] In particular, it gives the expectation value of $\mathcal{H}$ for closed shells, which are configurations $(N_1N_2\cdots)$ with only one state. By unitary transformations of the underlying fermion fields ($a_r^\dagger=\sum U_{rs}b_s^\dagger$), the n_r and T_r operators can only go to operators S_{rs} and T_{rs} coupled to $J=0$ and $T=0,1$, respectively (e.g., $n_r=a_r^\dagger\cdot a_r$ goes to $\sum U_{rs}U_{rt}b_s^\dagger\cdot b_t=\sum U_{rs}U_{rt}S_{st}$). Therefore the following must hold.[16]

Theorem.—There exists a decomposition $\mathcal{H}=\mathcal{H}_m+\mathcal{H}_M$ such that only $\mathcal{H}_m$ contributes to spherical HF calculations. $\mathcal{H}_m$ is written entirely in terms of unitary generators S_{rs} and T_{rs}.

The explicit form of the decomposition will be published elsewhere and will be made available on request.

Corollary.—By replacing expectation values by averages, HF variation can be extended to arbitrary configurations $(n_1n_2\cdots)$.[16]

Therefore we may assume that varying a good $\mathcal{H}_m$ produces an optimum field $\mathcal{H}_m(n)$ for each n and suggests a model space $\mathcal{M}$ spanned by configurations $(N_iN_jN_k\cdots n_rn_s\cdots)$ starting at $n=\sum n_r=0$, the core and extending to $n=N=\sum N_r$, the closed shell. The Hamiltonian that enters a shell-model calculation ($H=H_m+H_M$) is in first approximation the restriction of $\mathcal{H}$ to $\mathcal{M}$. We explain how its parameters "propagate" (a concept we borrow from the French), i.e., how they vary with n and how they are renormalized by states outside $\mathcal{M}$ (core polarization).

(II m) Propagation of H_m.—H_m has exactly the form of Eq. (1) with K_{rr} replaced by $\epsilon_r=K_{rr}+\sum N_{ir}V_{ir}$ (sum over occupied orbits i), but to incorporate observables as independent parameters we have to rewrite it[17,18] as

$$H_m=\mathcal{C}+\sum\Omega_r\eta_r+\sum_{r<s}\Omega_{rs}W_{rs}+\sum_{r\le s}\tau_{rs}b_{rs}\,,$$
$$\Omega_r=\left(\frac{n_r}{N_r}-\frac{n_1}{N_1}\right)N_r\,, \qquad (2)$$
$$\Omega_{rs}=\frac{N_{rs}}{2}\left(\frac{2n_{rs}}{N_{rs}}-\frac{n_{rr}}{N_{rr}}-\frac{n_{ss}}{N_{ss}}\right).$$

We have $\Omega_r=0$ at $n=0,N$, $\Omega_{rs}=\tau_{rs}=0$ [see Eq. (1)] at $n=0,1,N,N-1$. Furthermore, Ω_{rs} and τ_{rs} are invariant under $n_r\to\bar{n}_r$ and Ω_r changes sign. These properties explain the power of Eq. (2).

$\mathcal{C}=E+\epsilon n+Wn(n-1)/2$, with $E=\sum(K_{ii}N_i+V_{ij}\times N_{ij})$, $\epsilon=\sum N_r\epsilon_r/N$, $W=2\sum N_{rs}V_{rs}/N(N-1)$, is the total centroid. All quantities depend on n, e.g., $\mathcal{C}(0)=E(0)$ is the energy of the core, but in general $E=E(n)$ is the energy of the occupied orbits. The minimal parametrization we choose is $\mathcal{C}=\mathcal{C}(n,4)$, a polynomial of third order in n that for $n=0,N,1,N-1$ reproduces the core, closed-shell energies, and the single-particle and single-hole centroids, respectively (all observables).

$\eta_r=\epsilon_r-\epsilon+(n-1)W_r$, with $W_r=\sum(N_r-\delta_{rs})(V_{rs}-W)/(N-2)$, are the central-field splittings (note $\sum N_r\eta_r=0$). The minimal parametrization is $\eta_r(n,2)$, a linear form that reproduces the single-particle ($n=1$) and single-hole ($n=N-1$) splittings.

$W_{rs}=V_{rs}-W_r-W_s-W$ and b_{rs} are not directly observable. The minimal choice in this case follows hints from work in the fp shell[5] and it involves correcting the KLS values according to $W_{rs}=W_{rs}(\mathrm{KLS})+W_{rs}^0(X)$ and $b_{rs}=b_{rs}(\mathrm{KLS})+Y+2(\delta_{rs}-1)Z$, where W_{rs}^0 is the W_{rs}-type centroid of the monopole operator $X\sum(n_{rs}-n_{rr})$ $(r<s)$.

The minimal (or standard) parametrization we have described involves only three nonobservables (X,Y,Z). Physics may dictate more general forms as we shall see.

(II M) Propagation and core polarization in H_M.—The most conservative assumption about H_M is that matrix elements are calculated in an oscillator field common to all orbits (defined ideally by $\mathcal{H}_m$ variation). To relate its frequency $\hbar\omega$ (MeV) to the mean-square radius $\langle r^2\rangle^{1/2}$ (fm) we use[19]

$$\hbar\omega=40(a+bn)/\langle r^2\rangle(c+n)\,, \qquad (3)$$

where $(a,b,c)=(6,2.5,4)$ in the p shell and $(36,3.5,16)$ in the sd shell. For heavier regions the estimate $\hbar\omega=34.6A^{1/3}\langle r^2\rangle^{-1}$ (i.e., $40A^{-1/3}$ for $\langle r^2\rangle^{1/2}=0.93A^{1/3}$) should be sufficient. The behavior of H_M as a function of ω (and hence $\langle r^2\rangle$ and n) follows from $W_{rstu}^{JT}(\omega)\cong W_{rstu}^{JT}(\omega_0)\omega/\omega_0$, which holds fairly well for KLS. To account for core polarization we argue that in the first approximation it should affect the width of the eigenvalue distribution in $\mathcal{M}$ and we incorporate it through two multiplicative parameters λ_T. This is, of course, no substitute for the sophisticated calculations now possible,[20] but it is consistent with *monopole*-level *corrections* that must precede core-polarization *improvements* of $\mathcal{H}$. Separating the $T=0$ and 1 parts of H_M and incorporating ω dependence we end up with

$$H_M=\frac{\omega(n)}{\omega_0}\lambda_0\left(H^0+\frac{\lambda_1}{\lambda_0}H^1\right). \qquad (4)$$

It should be stressed that $\omega(n)$ is an observable through Eq. (3) and, therefore, involves no free parameters.

(III) Results: p and sd shells.—We have selected the free parameters through a least-squares fit to the (Coulomb-corrected) absolute energies of 179 states in the sd shell and 41 states in the p shell. The evolution of the root-mean-square deviations (RMSD) can be found in Table I. For the Cohen and Kurath[21] (CK) and Wildenthal[9] (W) interactions we have extracted the $\mathcal{C}$ centroid and replaced it by a $\mathcal{C}(n,6)$ form. For KLS we have fixed $\lambda_0=1$, $\lambda_1=1.4$ (sd), 1.2 (p). The uncertainties on λ_T are less than 10%. NP (no parameters) incorporates $\mathcal{C}(n,4)$ and $\eta_r(n,2)$ in Eq. (1).

S$\omega(v)$ (standard with polynomials of order $v-1$ for ω) brings in only X,Y,Z as free parameters for b_{rs} and W_{rs} in Eq. (1). The drop in RMSD between the con-

TABLE I. Root-mean-square deviations in keV for different calculations in the *sd* and *p* shells. See text.

	sd	*p*
W-CK	235	−605
NP	2500	1800
Sω(1)	883	920
Sω(2)	486	913
Sω(3)	475	913
Sω(4)	445	739
Sω(5)	443	700
Sω(6)	443	692
Sω(7)	441	674
SVω(1)	832	703
SVω(7)	399	380
FP	285	290

stant $\omega(1)$ and linear $\omega(2)$ forms and the stabilization after $\omega(4)$ in the *sd* shell need no comment. The physical origin of the effect clearly shows in Fig. 1 for $\omega(4)$. In the *p* shell the calculated ω is more complicated and not as convincing.

For SV$\omega(v)$ [standard variations with $\omega(v)$], we incorporate as free parameters some of the observables. In this case we allow variation for η_r and $\bar{\eta}_r$. In the *sd* shell we do not learn much. In the *p* shell the gain is spectacular and Fig. 2 for $\omega(7)$ is now quite satisfactory: The improvement with respect to S$\omega(7)$ comes from a smaller η_r (the $p_{1/2}$-$p_{3/2}$ splitting, intermediate between CK and experiment). Although this amounts to *p*-shell idiosyncrasy, there is a general point to be made: With the (mild) exception of $\mathcal{C}(n,4)$, Sω and SVω amount to *constant* ω for the energies which is not very consistent if ω turns out to have the aspect of Figs. 1 and 2. It is nice to have very few parameters but if the physics commands greater freedom, we must take it.

For FP (full propagation), we come back to experimental values for the observables but allow for $\mathcal{C}(n,6)$ and $\eta_r(n,6)$ forms. Furthermore, all W_{rs} $(r\neq s)$, b_{rr}, and $\sum b_{rs}$ $(r<s)$ are left to vary freely and propagate linearly. At this stage we enter the realm of high-quality

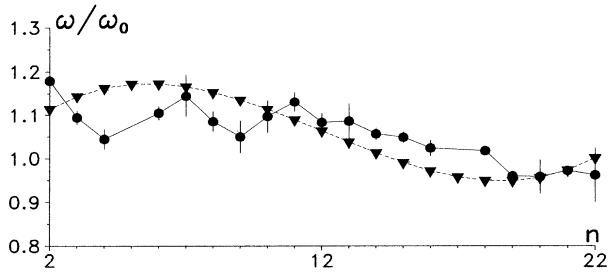

FIG. 1. Experimental (Ref. 26) Eq. (3) (circles and error bars) and calculated values of ω/ω_0 for S$\omega(4)$ in the *sd* shell (triangles) $\hbar\omega_0=11$.

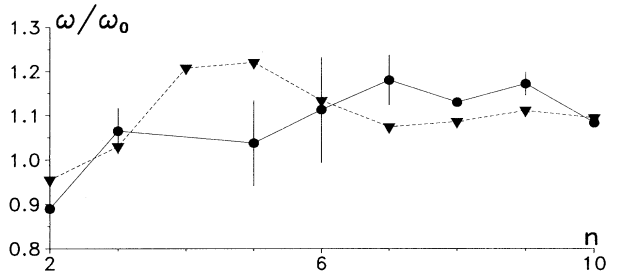

FIG. 2. Experimental (Ref. 26) Eq. (3) (circles and error bars) and calculated values of ω/ω_0 for SV$\omega(7)$ in the *p* shell (triangles) $\hbar\omega_0=13$.

spectroscopy and simultaneously explore saturation properties. Details will be given elsewhere.[22]

There are sources of uncertainty in the comparisons of Figs. 1 and 2: Eq. (3) may be naive, radii at fixed *n* may be *T* dependent (especially when deformation is present), and the λ_T parameters may be *n* and *T* dependent. However, these uncertainties are far from sufficient to cast doubts on a crucial result: *Spectra dictate choices of radii close to the experimental ones.* It should be noted that the *W* interaction yields RMSD=255, 235, and 215 keV for $\omega=\omega(2)$, $\omega=[18/(16+n)]^{0.3}$, and $\omega=\omega(6)$, respectively. The fact that a power law for ω is of no use in the *p* shell has led Van Hees, Booten, and Glaudemans[23] to introduce three-body forces that produce a drop in RMSD similar but smaller than those in Table I. It is an open question whether these results mock saturation effects or amount to genuine rank-3 forces.

(III) Results: N=50,82 isotones, Z=28,50 isotopes.—In these regions, SV$\omega(1)$ is sufficient to illustrate the luxuries we can afford with a realistic interaction.

(i) We select the ground states of even nuclei and the one-quasiparticle states of odd ones and do a seniority $v=0$ and 1 calculation (Table II). The values of η_r and $\bar{\eta}_r$ always come close to the experimental ones when these are known.

(ii) Having fixed the parameters, we increase v to 2,3,4,5, etc., and notice that v is a *very* good quantum number and that *many* states come quite naturally at observed positions to within the RMSD in Table II.

TABLE II. Root-mean-square deviations in keV for 0- and 1-quasiparticle fits in different isotone and isotope families. See text.

	λ_1	RMSD	$\hbar\omega_0$
$N=50$	1.35	160	9
$N=82$	1.35	128	7.9
$Z=28$	1.50	194	10.0
$Z=50$	1.40	129	8.4

Spectroscopy in the $N=82$ region is simply excellent.[22] For $N=50$, the results compare well with those of Ji and Wildenthal[24] except that our calculation misses a few levels they fit, brings the $g_{9/2}$ orbit at least 1 MeV lower, and conserves seniority better. The Ni and Sn isotopes are quite satisfactory in spite of a systematic discrepancy: For low n the first 2^+ state comes too high (up to 600 keV in Ni, 300 keV in Sn). Problems of this sort should be put to the *credit* of the interaction for signaling trouble in the calculation. In the case of Ni we know it must come from coupling to low-lying states in ^{56}Ni.[5] For Sn, the situation is bound to be similar: In general, $N=Z$ cores are easier to polarize than those with neutron excess and demand careful treatment.

Propagation plays a minor role in these regions, except through the linear behavior of the single-particle field, which is compatible with a constant two-body force.

In conclusion, the separation theorem provides the framework that dictates the necessary steps to enforce good monopole behavior. Some of them have been described previously[18,25] and now we propose a consistent implementation with bare forces and very few parameters, that stresses the influence of radii in light nuclei. Realistic forces are quite adequate for spectroscopic work provided saturation properties are taken care of.

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