The Nuclear Monopole Hamiltonian

J. Duflo[a] and A. P. Zuker[b]

(a) Centre de Spectrométrie Nucléaire et de Spectrométrie de Masse (IN2P3-CNRS) 91405 Orsay Campus, France

(b) IRES, Bât27, IN2P3-CNRS/Université Louis Pasteur BP 28, F-67037 Strasbourg Cedex 2, France

(November 5, 1998)

The monopole Hamiltonian H_m is defined as the part of the interaction that reproduces the average energies of configurations. After separating the bulk contributions, we propose a minimal form for H_m containing six parameters adjusted to reproduce the spectra of particle and hole states on doubly magic cores. The mechanism of shell formation is then explained. The reliability of the parametrization is checked by showing that the predicted particle-hole gaps are consistent with experimental data, and that the monopole matrix elements obtained provide the phenomenological cure made necessary by the bad saturation and shell properties of the realistic NN interaction. Predictions are made for the yet unobserved levels around ^{132}Sn, ^{22}O, ^{34,42}Si, ^{68,78}Ni, ^{100}Sn and for the particle-hole gaps in these nuclei.

21.10.Pc, 21.30.+y, 21.60.Cs

There used to be two kinds of fermion systems: those with many particles and those with few. Nuclei occupied an uneasy middle ground—too large to be studied with the precision of coordinate space methods, and too small to take advantage of the simplicity of momentum space—and a new representation had to be invented for them: the harmonic oscillator (HO). As Helium droplets and metallic clusters have increased the variety of finite self-bound systems, some typical features of the HO representation may become of general interest, in particular the origin of shell structure, which appears under a new light as a natural byproduct of the method we present to circunvent the problem of the bad saturation properties of the potentials derived from NN data.

Recent exact results [1,2] for $A \leq 8$ indicate that an apparently perfect potential, supplemented by a three body term produces excellent spectroscopy, but has problems with the absolute binding and symmetry energies and the spin-orbit splittings. Very much the same happens in shell model work, where sophisticated derivations of the effective interaction [3] fail to reproduce the closed shell nature of ^{48}Ca. This problem has been kwown for long, and the solution is simply to readjust some centroids of the interaction [4], defined in terms of the two body matrix elements as $V_{kl}^{xx'} = \sum_J (2J+1) V_{klkl}^{Jxx'} / \sum_J (2J+1)$, where xx' stand for neutrons or protons in orbits kl. Much work has gone into deducing these important parameters directly from the data (see e.g. [5], and references therein), but it was not widely realized (or accepted) that the *only* problem of the realistic interactions is associated with centroids. If these are replaced by fitted ones, the reults are excellent [6–8]. Our purpose is to recast the part of the Hamiltonian given in terms of centroids, in such a form that it can be deduced directly from experimental data. Therefore, whatever has to be fitted is fitted once and for all, and not case by case.

First we note that matrix elements for a potential of short—but non zero—range scale as the oscillator frequency $V'(\omega)_{klmn} \cong \frac{\omega}{\omega_0} V(\omega_0)_{klmn}$ which is the analogous to the inverse-volume scaling in box quantization. (Here, and in what follows, unprimed quantities denote operators stripped of their $\hbar\omega$ factor.) Now assume that "somehow" the saturation problem has been solved, and we are given an effective potential that scales as ω. This cannot be entirely true, because then the competition between potential and kinetic energy ($K' = \hbar\omega/2 \sum_p (p+3/2) m_p$, m_p is the number of particles in HO shell p) would lead to a trivial equilibrium at $\hbar\omega = \infty$ or 0. However, most realistic G-matrix elements obey quite nicely this law [6,9]. Therefore, we must identify the few that do not. To do so, we separate $H = H_m + H_M$, so that H_m, the monopole Hamiltonian, contains all quadratic (two body) forms in the scalar products $a_r^+ \cdot a_s$. Its diagonal part is then given in terms of the centroids introduced above, and the number operators m_k^x of orbit k in fluid x.

$$H_m^d = \frac{1}{2} \frac{\hbar\omega}{\hbar\omega_0} \sum_{k,l,x,x'} V_{kl}^{xx'} m_k^x (m_l^{x'} - \delta_{kl}\delta_{xx'}). \tag{1}$$

Calling $D_p = (p+1)(p+2)$, the degeneracy of HO shell p, the matrix element we are after must be the coefficient of the collective monopole-monopole interaction, $W' = \hbar\omega (\sum_p (m_p/\sqrt{D_p})^2$, since it is the *only* contribution to H_m^d that goes as the total number of particles A [10,11]. Therefore, it is here that the $\hbar\omega$ scaling must be supplemented by a more complicated dependence. The ideal solution we have assumed must be such that the kinetic energy is cancelled. This we do by choosing as first contribution to H_m^d the combination $\hbar\omega(4K - W)/4$, which cancels exactly to order $A^{1/3}$ but, as we shall see, produces the basic shell effect . The bulk (A), and surface ($A^{2/3}$) terms, that the solution must also provide need not concern us here, and from now on we use H_m^s to denote the subtracted H_m^d. Now it is safe(r) to rely on ω scaling, and since [12], $\omega \propto A^{1/3}/\langle r^2 \rangle \equiv 1/\rho$, we affect all the terms by the scaling factor $1/\rho$

$$\rho = (A^{1/3}(1 - (2T/A)^2) e^{(3.5/A)}, \tag{2}$$

obtained using a very accurate fit to the data ($\langle r^2\rangle = 0.9\rho A^{1/3}$ a variant of those in [13]). The factor $1/\rho$ will be tacitly assumed in all that follows.

The strategy to determine H_m^d follows from the fact that its expectation value for any state is the average energy of the configuration to which it belongs (a configuration is a set of states with fixed m_k^x for each orbit). In particular H_m^d reproduces the exact energy of closed shells (cs) and single particle (or hole) states built on them ($(cs)\pm 1$), since for this set ($cs \pm 1$) each configuration contains a single member. As a consequence it is uncontaminated by direct configuration mixing and we have chosen as input data the spectra around doubly magic cores.

Technically, the problem is to recast H_m^d in a form that isolates the few pertinent parameters. The tool [6,14] consists in replacing the set of m_i operators in a major shell, by m_p and $\Gamma_{ij} = (m_iD_j - m_jDi)/(D_i + D_j)$, with j arbitrarily chosen. D_i is the degeneracy of orbit (or group of orbits) i. In turn, the m_p could be regrouped to single out the total $m = A$. For the quadratic forms we have (schematically) $m(m-1), (m-1)\Gamma$ and $\Gamma\Gamma$ terms, which behave as constant, one-body, and two-body respectively for fixed m.

Now we present the operators we (or rather the data) have selected. Two of them behave as one body: $l\cdot s$ and $l\cdot l$, and there are four two-body groups that account for the modifications brought about by the "intruder" orbit at the EI (Extruder-Intruder, i.e., 6,14,28...) closures. To fix ideas, note that the $(cs)\pm 1$ states associated to ^{40}Ca are quite different from those in ^{48}Ca. Their experimental energies are given in the first row of table I, where the labels of the four groups are also shown: znc, ffc, ffi, zni. They correspond to the cases in which the intruder and the orbits it acts upon are in the same or different fluids (ff or nz) and the same or different major shells (i or c).

The notation for orbits or groups is: p, the full shell; $l = l_> + l_<$, the spin orbit partners, but $q = p_> + p_<$ ($p_>$ is the extruder-intruder, i.e. the largest orbit that migrates to shell $p-1$ to form the EI shell). Then, $R = p - p_>$, $r = p - q$, and finally $\bar{l} = p - l$.

The linear operators are defined through

$$d_p = \sum_l \frac{l+1/2}{p+2}\Gamma_{l_>l_<}, \qquad d = l\cdot s = \sum_p d_p \tag{3a}$$

$$e_p = \sum_l \frac{l(l+1)\Gamma_{l\bar{l}}}{D_p}, \qquad e = l\cdot l = \sum_p \frac{p-3}{\sqrt{D_p}}e_p. \tag{3b}$$

There is also a d' operator, identical to d, but restricted to act on r orbits only. Similarly, for e'_p, where now $\bar{l} = r - l$. It can be checked that the $l\cdot l$ displacements are refered to their centroids: $(p+1)(p+3)/2$ for e_p, and $(p-2)(p+1)/2$ for e'_p. The quadratic operators are given by

$$zncv = \sum_{p\neq p', x\neq y} \frac{\Gamma^x_{p_>R}\Gamma^y_{p'_<r}}{(D_pD_{p'})^{1/4}}, \; znie = \sum_{p,x\neq y}\frac{m^x_{p>}e^y_p}{D_{p>}}, \tag{4a}$$

$$znie' = \sum_{p,x\neq y}\frac{e'^x_p\Gamma^y_{p>R}}{D_{p>}}, \quad ffce = \sum_{p\neq p',x}\frac{e^x_pe^x_{p'}}{(D_pD_{p'})^{1/4}}, \tag{4b}$$

$$ffis = \sum_{xp}\frac{m^x_{p>}}{D_{p>}}\left(\Gamma^x_{p>R} - \frac{p(D_p - m^x_p)}{(p+2)(D_p-1)}\right). \tag{4c}$$

There is also a $znid$ operator of the same form as $znie$. The subtraction in $ffis$ ensures that the operator is two-body. The denominators are chosen to have splittings of order unity so that they become $O(A^{-1/3})$ when the $1/\rho$ factor is reintroduced.

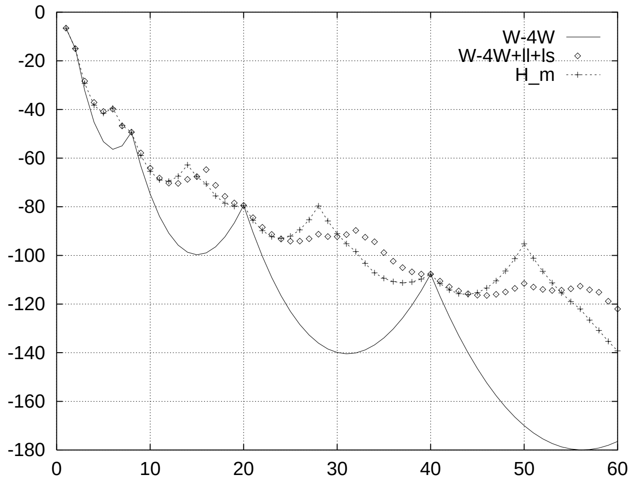

FIG. 1. Monopole shell effects in the binding energies of $T=0$ nuclei

The combination (we use the convention of positive binding energies, all quantities in MeV)

$$\begin{aligned}\rho H^s_m &= [9.53(W - 4K + 2d + 2e) - 1.77(2d + 2d')\\ &+3.63(ffce + 2zncv) + 7.32ffis\\ &+8.35(znie - znie') - 2.19znid],\end{aligned} \tag{5}$$

yields a deviation (rmsd) of 221 KeV, in a fit to the experimental excitations adopted in table I. To within 2 keV, the rmsd is the same for nuclei with $A > 60$ and $A < 60$.

Fig. I shows how $W - 4K$ produces the HO closures. The coefficient of K, 38ρ, which also turns out to be the shell gap, comes spontaneously close to the $\hbar\omega = 40\rho$ estimate. Everything happens as if the naive HO picture were true. The addition of the $l\cdot s$ and $l\cdot l$ terms very much erases the HO closures but *does not produce the* EI ones, which only come about through the action of the two-body terms.

Before inspecting H^s_m in more detail, let us check its reliability through the shell gaps (not included in the fit) given at the bottom of Table I. We have added to H^s_m

a symmetry energy $-22[4T(T+1)](1-1.82/\rho)/A$ taken from [11], but reducing the volume term by some 6.5 MeV produced by $W-4K$. At first sight, the agreement with the data [16] seems rather random: the gap in ^{12}C is some 6 MeV too small, in ^{48}Ca it is about perfect, and 1 MeV too large in ^{56}Ni. *But*, these are precisely the contributions of the correlation energies coming from accurate shell model work (in [6,7,15] respectively). The omens are good but more calculations are necessary. At the moment eq. (5) has been tested in the pf shell—where it yields very good spectroscopy [18], and cures the defects of the KB3 interaction [7]—and through Monte Carlo calculations in the full *sd*-*pf* shell [17], which cannot provide high precision, but demonstrate its capacity to cope very well with very large spaces.

The centroids of $(cs)\pm 1$ spectra are by definition inmune from correlations, but not easy to extract from experiment [19], and the numbers given in Table I are often those of the main peak. In view of uncertainties that may be easily of some 300 keV per level, the fit seems to do quite well, and by examining term by term the action of eq. (5), we shall have an idea of the weight to attach to a given prediction.

$d\equiv l\cdot s$. No problem here. The second term is a mild comment.

$e\equiv l\cdot l$ changes sign at $p=3$. Strange. See next.

$ffce+2zncv$. The 2 $s_{1/2}$ orbit is the great troublemaker: responsible for halos, for the change in sign in $l\cdot l$, it also comes too low in ^{47}Ca, about right in ^{47}K and too high in ^{55}Ni . There is no possible monopole combination that can place the three levels at their observed positions, only correlations can do it. By systematics we expect in $A=99$ a smaller observed splitting between 3 ($p_{1/2}$) and 44 ($g_{9/2}$) than in Table I. However, the overall action of the term is very sound. In particular $zncv$ does very well for the recently observed 13-23 ($p_{3/2}$-$f_{5/2}$) splittings [20]: 0.53 MeV in ^{71}Cu, and 0.17 MeV in ^{73}Cu, it predicts 0.5 and 0.1 MeV respectively. Similar story in Sb for the 24-34 pair.

$ffis$ by itself turns ^{48}Ca into a closed shell. *It is this term that the realistic interactions conspicuously fail to produce.* Very good test for a three-body force.

zni... this is a complicated mixture that the realistic interactions seem to reproduce reasonably, although some repulsion between the $p_>$ and R orbits is missing (same effect as for $ffis$, but weaker). This term needs revisiting, but its effects are quite sound, in particular, they reproduce the radical change of spectra between ^{48}Ca and ^{56}Ni.

Though the form of H_m^s was suggested only by the lighter nuclei, it does quite well around ^{132}Sn and ^{208}Pb. The only complaint could come from the big ($p_>$) orbits, but it is well known that they are the most affected [21] by particle-vibration coupling. Therefore, we think that our prediction for the level orderings in ^{133}Sn is quite strong, even if it contradicts the (somewhat speculative) experimental assignment [22] in which the first excited states are inverted with respect to ours.

The key step of our method is the separation of bulk and shell effects achieved by cancelling the kinetic energy against the collective monopole interaction—a concrete example of Strutinsky famous theorem—that should apply to other selfbound systems. The way the HO closures evolve into the observed ones then depends on the system, but the nuclear example could serve as a guide for modeling them.

A preliminary version of this work was completed during the stay of AZ at the Institute for Nuclear Theory at the University of Washington, whose hospitality and excellent working conditions are thankfully acknowleged.

---

[1] B.S. Pudliner, V.R. Pandharipande, J. Carlson, S. Pieper and R. W. Wiringa Phys. Rev. C **56**, 1720 (1997).
[2] R. W. Wiringa in 15th Intl. Conf. on few body problems, Groningen (1997)
[3] M. Hjorth-Jensen, T.T.S. Kuo and E. Osnes, *Phys. Reps.* **261**, 125 (1995).
[4] E. Pasquini, Ph.D. thesis, Report No. CRN/PT 76-14, Strasburg, 1976. E. Pasquini and A. P. Zuker in *Physics of Medium Light Nuclei*, Florence, 1977, edited by P. Blasi and R. Ricci (Editrice Compositrice, Bologna, 1978).
[5] S. Pittel *et al.* Pys. Rev. C **48**, 1050 (1993)
[6] A. Abzouzi, E. Caurier et A.P. Zuker, Phys. Rev. Lett. **66**, 1134 (1991).
[7] G. Martínez-Pinedo, A.P. Zuker, A. Poves and E. Caurier, Phys. Rev. C **55**, 187 (1997)
[8] A.P. Zuker, in Contemporary Shell Model, edited by X.W. Pan (Springer Lecture Notes 482, 1997)
[9] G. Bozzolo, A. Klar and J.P. Vary, Phys. Rev. C **29**, 1069 (1984)
[10] M. Dufour and A.P. Zuker, Phys. Rev. C **54**, 1641 (1996)
[11] J. Duflo and A.P. Zuker, Phys. Rev. C **52**, R23 (1995)
[12] A. Bohr and B. Mottelson, *Nuclear Structure* vol I (Benjamin, Reading, 1964).
[13] J. Duflo, Nuc. Phys. **A576**, 29 (1994)
[14] A. P. Zuker, Nuc. Phys. **A576**, 65 (1994)
[15] E. Caurier, G. Martínez-Pinedo, A. Poves and, A.P. Zuker Phys. Rev. C **52**, R1736 (1995)
[16] G. Audi and A.H. Wapstra, Nuc. Phys. **A565**, 1 (1993)
[17] D. Dean *et al.*, submitted to Phys. Rev. **C**
[18] F. Nowacki, private communication.
[19] Electronic version of Nuclear Data Sheets, http://www.dne.bnl.gov/nndc.html.
[20] S. Francho *et al.*, Phys. Rev. Lett. **81**, 3100 (1998)
[21] I. Hamamoto, Phys. Rep. **10 C**, 63 (1974)
[22] P. Hoff *et al.*, Phys. Rev. Lett. **77**, 1020 (1996)

TABLE I. Excitation energies, ngaps (2BE(Z N)-BE(Z N+1)-BE(Z N-1)) and zgaps (2BE(Z N)-BE(Z+1 N)-BE(Z-1 N)). Orbits labeled by $j-1/2$ p, so 12 and 2, say, stand for $j=3/2$ and $j=1/2$ in the $p=2$ shell, (i.e. $0d_{3/2}$ and $1s_{1/2}$). In first row of upper boxes: ground state orbit, element, Z N. Experimental (parenthesis for those not included in the fit) and calculated values given with two and one decimals respectively.

12	Ca	**20 19**	33	Ca	**20 21**	2	K	**19 28**	33	Ca	**20 27**	13	Ca	**20 29**	33	Sc	**21 28**
2	1.9	2.40	13	1.9	2.00	12	0.2	0.36	12	2.6	2.58	3	1.9	2.00	13	4.0	4.00
22	6.2	6.00	3	3.8	4.00	22	5.7	5.70	2	3.2	2.60	23	3.9	4.00	3	5.5	5.50
1	13.7		23	5.9	6.00	1	14.2		22	8.6	8.00	44	4.9		23	5.0	4.70
			44	7.5				znc			ffc	24	8.3	ffi	44	8.2	zni
1	O	**8 7**	22	O	**8 9**	1	N	**7 14**	22	O	**8 13**	2	O	**8 15**	22	F	**9 14**
11	6.3	6.20	2	0.8	0.87	11	6.7		1	4.1		12	5.7		2	3.1	
0	22.7		12	6.2	6.00	0	27.5		11	10.4		33	7.4		12	5.3	
			33	8.4	8.97							13	10.4		33	9.1	
22	Si	**14 13**	2	Si	**14 15**	22	Al	**13 20**	12	Si	**14 19**	33	Si	**14 21**	2	P	**15 20**
1	4.8	4.20	12	2.0	1.40	1	6.0		2	2.0		13	2.7		12	2.0	2.39
11	10.5		33	4.5	4.00	11	11.8		22	6.7		3	4.8		33	5.6	
			13	8.3					1	13.5		23	5.6		13	8.1	
												44	8.1				
22	Al	**13 28**	33	Si	**14 27**	13	Si	**14 29**	2	P	**15 28**	33	Ni	**28 27**	13	Ni	**28 29**
1	7.5		12	2.3		3	2.1		12	0.1		2	1.4	2.90	23	1.0	0.77
11	13.5		2	3.0		23	3.0		33	4.2		12	3.1	3.20	3	1.4	1.11
			22	9.1		44	4.4		13	9.3		22	8.1		44	3.3	3.50
						24	8.8								24	7.1	
33	Co	**27 40**	3	Ni	**28 39**	44	Ni	**28 41**	13	Cu	**29 40**	33	Co	**27 50**	3	Ni	**28 49**
12	3.5		23	0.4		24	3.0		3	1.3	1.10	2	3.1		44	0.1	
2	4.1		13	1.3		4	4.2		23	1.0	1.21	12	4.9		13	1.4	
22	9.1		33	6.7		34	4.7		44	3.7		22	9.7		23	1.8	
			12	11.3		14	5.3		24	6.9					33	8.1	
						55	6.2										
24	Ni	**28 51**	23	Cu	**29 50**	23	Zr	**40 39**	44	Zr	**40 41**	3	Y	**39 50**	44	Zr	**40 49**
4	1.3		13	1.1		3	0.0		24	2.2		13	1.2	1.51	3	0.4	0.59
34	1.8		3	2.5		13	1.9		4	3.3		23	2.2	1.75	23	2.0	1.45
14	2.4		44	3.3		33	5.6		14	4.4		33	6.8		13	1.6	1.74
55	3.0		24	8.8		12	10.3		34	5.2		12	12.6		33	7.5	
35	7.3								55	6.6							
24	Zr	**40 51**	44	Nb	**41 50**	3	Sn	**50 49**	24	Sn	**50 51**	44	In	**49 82**	14	Sn	**50 81**
4	1.2	1.20	24	4.2		44	1.0		34	0.5		3	0.1	0.35	4	0.3	0.33
14	2.1	2.00	34	4.7		13	1.2		4	0.8		13	1.2		55	0.9	0.24
34	3.0	2.70	4	5.0		23	3.4		14	1.6		23	3.8		24	1.6	1.52
55	3.6		14	5.9		33	7.7		55	2.4		33	7.8		34	2.4	2.43
35	6.9		55	7.4					35	6.1					44	8.2	
35	Sn	**50 83**	34	Sb	**51 82**	4	Tl	**81 126**	5	Pb	**82 125**	46	Pb	**82 127**	45	Bi	**83 126**
45	1.2		24	1.3	0.96	14	0.5	0.35	25	0.5	0.57	56	0.9	0.78	35	1.2	0.90
15	2.3		55	2.7	2.79	55	1.2	1.35	15	0.7	0.90	26	1.2	1.57	66	2.2	1.60
25	2.4		14	2.9	2.71	24	1.9	1.68	66	1.6	1.63	77	1.9	1.42	15	2.9	3.12
66	2.3		4	2.9		34	4.4	4.60	35	2.1	2.34	36	2.3	2.49	25	2.6	2.83
5	3.0		35	7.8		44	7.9		45	3.0	3.41	6	2.0	2.03	5	3.6	3.60
46	6.1								55	8.2		16	2.6	2.54	46	7.0	
												57	5.3				

	C	**6 6**		C	**6 8**		O	**8 8**		O	**8 14**		O	**8 20**		Si	**14 14**
ngap	8.0	13.78	ngap	4.9	6.96	ngap	6.5	11.52	ngap	4.1	4.11	ngap	2.9		ngap	7.1	8.71
zgap	8.4	14.01	zgap	7.9	10.62	zgap	7.0	11.53	zgap	7.6	9.99	zgap	10.5		zgap	7.4	8.84
	Si	**14 20**		Si	**14 28**		Ca	**20 20**		Ca	**20 28**		Ni	**28 28**		Ni	**28 40**
ngap	3.9	5.06	ngap	6.2		ngap	5.2	7.28	ngap	4.8	4.80	ngap	7.4	6.39	ngap	3.2	2.85
zgap	6.5	6.55	zgap	8.7		zgap	5.5	7.24	zgap	5.4	6.18	zgap	7.6	6.47	zgap	6.7	5.91
	Ni	**28 50**		Zr	**40 40**		Zr	**40 50**		Sn	**50 50**		Sn	**50 82**		Pb	**82 126**
ngap	5.9		ngap	3.8		ngap	4.7	4.77	ngap	6.0		ngap	4.3	4.89	ngap	3.0	3.43
zgap	8.0		zgap	4.0		zgap	1.3	2.00	zgap	6.2		zgap	5.7	6.07	zgap	3.7	4.20