Microscopic mass formulae

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By assuming the existence of a pseudopotential smooth enough to do Hartree-Fock variations and good enough to describe nuclear structure, we construct mass formulae that rely on general scaling arguments and on a schematic reading of shell model calculations. Fits to 1751 known binding energies for N,Z ≥ 8 lead to RMS errors of 614 keV with 14 parameters and 388 keV with 28 parameters. The latter is easily reduced to a 20 parameter form at 423 keV.

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Calculations of nuclear masses reflect the traditional cleavage between local methods of shell model origin and global ones, in which semiclassical arguments play an important role. Out of the ten contributions to the 1986-1987 mass predictions\textsuperscript{[1]}, two are simply numerical, three follow Garvey-Kelson lines, and five incorporate a Bethe-Weizsäcker liquid drop (LD) formula as basic ingredient. The earlier work of Liran and Zeldes\textsuperscript{[2]} is a shell model approach and the recent Thomas-Fermi (ETFISI) calculations of the Montréal-Brussels group\textsuperscript{[3]} are definitely global but belong to a special category in that the number of parameters is truly small (9) and the LD form comes as output.

At present, only the local formulae of Masson and Jänecke\textsuperscript{[1]} can go below RMS errors of 400 keV but they need hundreds of parameters and cannot reach safely the drip-lines as demanded by calculations of r-processes nucleosynthesis. The droplet (FRDM)\textsuperscript{[1,4]} and ETFISI\textsuperscript{[3]} mass tables are designed to extrapolate efficiently but they differ in hundreds of parameters and cannot reach safely the drip-lines as demanded by calculations of r-processes nucleosynthesis.

To obtain some improvements we propose to abandon the local-global dichotomy and go back to fundamentals. The only assumption we shall make is that there exits a nucleon-nucleon (NN) pseudopotential smooth enough to do Hartree-Fock (HF) calculations and good enough to explain nuclear structure. The pseudopotential cannot be identical to - although we expect it to resemble - the bare HF calculations and good enough to describe nuclear structure. We construct mass formulae that rely on general scaling arguments and on a schematic reading of shell model calculations. Fits to 1751 known binding energies for N,Z ≥ 8 lead to RMS errors of 614 keV with 14 parameters and 388 keV with 28 parameters. The latter is easily reduced to a 20 parameter form at 423 keV.

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The multipole Hamiltonian $\mathcal{H}_M$ contains all other terms (pairing, quadrupole, etc). It is therefore responsible for correlations, while $\mathcal{H}_m$ is in charge of saturation properties.

The $\mathcal{H}_m + \mathcal{H}_M$ separation is a rigorous result whose proof is sketched in \textsuperscript{[5]} and given in general in \textsuperscript{[6]}. It was used in \textsuperscript{[7]} to demonstrate that once $\mathcal{H}_m$ is treated phenomenologically, a parameter-free $\mathcal{H}_M$ derived from realistic interactions is sufficient to provide high quality shell model spectroscopy in all regions where exact diagonalizations are feasible (RMS errors below 300 keV in the $p$ and $sd$ shells, below 200 keV in the N = 50,82 isotones and Z = 28,50 isotopes).

In shell model calculations, the full $\mathcal{H}$ is not directly used but replaced by a renormalized version $H = H_m + H_M$ adapted to finite spaces in regions bounded by magic closures. Then $H_M$ is taken to reproduce exactly the corresponding $cs = \pm 1$ states.

Although our ultimate aim would be to discover $\mathcal{H}_m$, in this paper we propose a simpler, and probably necessary first step which is the determination of the gross features of $\mathcal{H}_m$ by including it as basic ingredient in a mass formula. Let us assume then that we have some $H = H_m + H_M$, ready for shell model calculations:

$$H = \sum A_{kl}m_km_l + B_{kl}t_k.t_l + H_M$$

which is taken to be a strictly two body force by including in it the kinetic energy after elimination of the center of mass contribution. However, for simplicity we have omitted in eq.(2) the counter terms in $\delta_{kl}$ in eq.(1) (we have checked that their effect is negligible in the fits).

To obtain some clues about $H_m$ we reduce it to separable form by diagonalising the $A_{kl}$ and $B_{kl}$ matrices.
For \( A_{kl} \) we have

\[
\sum_{k,l} A_{kl} m_k m_l = \sum_{\mu} e_\mu (\sum_k m_k f_{k\mu})^2
\]

and borrow from [3] the result that a realistic force produces a strongly dominant \( e_0 \), whose eigenvector \( M \) has amplitudes

\[
f_{k0} = \left[ (p+1)(p+2) \right]^{-1/2} = D_p^{-1/2}
\]

where \( k \) belongs to the \( p \)-th harmonic oscillator shell of degeneracy \( D_p \).

Let us study this term. Setting \( m_p = n_p + z_p \), where \( n, z \) are number operators for neutrons (\( \nu \)) and protons (\( \pi \)), filling shells \( p_\nu \) and \( p_\pi \) up to some \( p_f \nu \) and \( p_f \pi \) Fermi level, we find:

\[
< M > = \sum_p m_p / \sqrt{D_p} \approx \frac{1}{2} [(3N)^{2/3} + (3Z)^{2/3}]
\]

where we have approximated \( \sqrt{(p+1)(p+2)} \approx p + 3/2 \), and used \( N = \sum n_{p\nu} = \sum (p_\nu +1) (p_\nu +2) \approx \frac{4}{3} (p_\nu +2)^3 \) and \( Z = \frac{1}{3} (p_f \nu +2)^3 \).

The eigenvalue \( e_0 \) must behave as a typical two body matrix element, which for a realistic force goes as

\[
V(\omega)_{klmn} \cong \frac{\omega}{\omega_0} V(\omega_0)_{klmn} + O(\omega^2)
\]

a result from ref. [3], but adding an \( O(\omega^2) \) correction warranted for large oscillator constant \( \omega \). Then we know that

\[
\frac{\hbar \omega}{\langle r^2 \rangle} = \frac{34.6 A^{1/3}}{40 A^{-1/3} + O(A^{-2/3})}
\]

where the leading term is the classical result [3] obtained with a standard mean square radius \( <r^2> = 0.86 A^{2/3} \). The \( O(A^{-2/3}) \) correction comes because the light nuclei are larger than the standard estimate. By combining eqs.(6) and (7) we obtain the scaling law \( \Gamma(A) = \Gamma A^{-1/3} + \gamma A^{-2/3} \), or its more flexible generalization

\[
\Gamma(A) = \left( \Gamma/R \right) (1 - \rho(\Gamma/R)) \quad , \quad R = R^2/A^{1/3}
\]

that we shall use for all amplitudes \( \Gamma(A) \) affecting operators \( \tilde{\Gamma} \). The form of \( R \) is left free to allow for the better estimate: \( <r^2> = 0.90 R^2 \), with \( R_c = A^{1/3} (1 - \xi (2T/A)^2)^{1/3} \), \( \xi = 0.42 \) [3].

For the leading monopole term we have from eqs.(5) and (8) \( \tilde{\Gamma} \Gamma(A) = \sum \frac{m_p}{\sqrt{D_p}} \omega_0 e_0 = O(A) + O(A^{2/3}) \).

This remarkable object goes asymptotically as volume plus surface LD terms and at the same time produces strong magicity at the harmonic oscillator (HO) closures, as can be checked by plotting \( \Gamma \) (or more precisely its expectation value ). To obtain the usually observed extruder-intruder (EI) closures we have to add spin-orbit (SO) effects and we rely on the diagonal construction (3) to propose a term orthogonal to \( M \) of the form \( S = \sum S_p N^{-1}_p \), where \( N_p \) is a normalization to be determined and

\[
S_p = pm_{jp} - 2m_{rp} = (\tilde{l}.s)_p.
\]

Here (refer to Fig.1) \( jp \) is the largest orbit in the \( p \)-th shell and \( rp \) regroups all the others. \( (\tilde{l}.s)_p \) is the operator that produces the same splittings as \( (l.s)_p \) and then collapses the \( r \)-orbits to their centroid value. The rationale for considering only two types of orbits is clear from Fig.1: we want to give top priority to shell formation (i.e. the cs part of the cs + 1 set ). The combinations of \( m_k \) operators other than \( m_j \) and \( m_r \) will contribute to subshell effects that we incorporate in \( H_M \) and treat later.
ho ei

\[ D_{p+1} \] \hspace{1cm} \[ r(p+1) \]

\[ D_p \] \hspace{1cm} \[ j(p) \]

\[ j(p) \] \hspace{1cm} \[ r(p) \]

\[ j(p) \] \hspace{1cm} \[ D_{\nu,\pi} \]

\[ D_J = 2(p+1) \] \hspace{1cm} \[ D_{\tau p} = p(p+1) \]

\[ D_{\nu,\pi} = D_p + 2 = D_V \] \hspace{1cm} \[ n_{\nu,\pi} = n_v = n_j(p+1) + n_{\tau p} \]

FIG. 1. HO and EI major shells.

Since \( M \) and \( S \) are symmetric combinations of (properly scaled!) \( m_p \) and \( S_p \) operators, the only other contributions we can include consistently must be symmetric in \( p \), i.e., sums of \( m_p^2 \) and \( S_p^2 \), again properly scaled. The arguments are exactly the same for the \( t \) operators.

Calling \( m_p = n_p + z_p \), \( t_p = |n_p - z_p| \), \( S_p = p(n_jp + z_jp - 2(n_{\tau p} + z_{\tau p}) \), and \( ST_p = p|n_jp - z_jp| - 2|n_{\tau p} - z_{\tau p}| \), we introduce the variables

\[
MA_p = \frac{m_p}{\sqrt{D_p}}, \quad SA_p = \frac{S_p}{2(p+1)}, \tag{10a}
\]

\[
MT_p = \frac{t_p}{\sqrt{D_p}}, \quad ST_p = \frac{ST_p}{2(p+1)} \tag{10b}
\]

In general \( A = N + Z \) and \( T = |N - Z|/2 \), but in combinations as above, they mean “isoscalar” and “isovector” respectively, while \( M \) stands for “master” and \( S \) for “spin-orbit”. The first part of Table 1 gives the 12 possible symmetric quadratics obtained with operators (10). \( F \) here stands for “full” and \( P \) for “partial”. All these operators will be affected by coefficients that scale as \( \Gamma(A) \) in eq.(8). The \( FC^T \) term is chosen to go as an ordinary \( \zeta l.s \) term with \( \zeta = O(A^{-2/3}) \). The other scalings then follow by symmetry. It could be argued that the \( S \) operators in eq.(10) should carry an extra \( O(p^{-1/2}) \) factor. This uncertainty is of little consequence. On the contrary the \( D_p^a \) factor is important and we shall let the fits decide in favour of \( a = 1/2 \).

### TABLE I. The operators \( \Gamma \) (called \( \Gamma \) here) in \( H_m, H_s \) and \( H_d \)

| \( H_m \) \( (T = |N - Z|/2) \) | \( H_s \) \( \bar{\nu} = \bar{\nu} + \bar{z} = D_n - z \) | \( H_d \) \( (n' = n - JU, \bar{n}' = \bar{n} + JU) \) | \( 4T(T+1)A^{-2/3} \) |
|-----------------|-----------------|-----------------|-----------------|
| \( \alpha = 1/2 \) | \( S2 = n\bar{n}D_{\nu}^{-1} + z\bar{z}D_{\pi}^{-1} \) | \( QQ^{0} = (n'\bar{n}'D_{\nu}^{-3/2} + \bar{z}'z'D_{\pi}^{-3/2})^2 \) |
| \( R_c = [A(1 - \xi(2T/A)]^{1/3} \) \( \xi = 0.42 \) | \( S3 = n\bar{n}(n - \bar{n})D_{\nu}^{(2\beta - 1)} + z\bar{z}(z - \bar{z})D_{\pi}^{(2\beta - 1)} \) | \( DK = 16 \) |

In addition to these terms \( H_m \), includes standard pairing \( (V_p) \) and Coulomb \( (V_c) \) contributions as well as a \( 4T(T+1) \) term whose presence is necessary.

If \( H_m \) has ensured shell formation, mostly of EI type, the variables that become important in modelling configuration mixing are \( n_v \) and \( z_v \), the number of valence particles in EI spaces of degeneracy \( D_v \) and \( D_{\pi} \) (see Fig.1). If we assume
a-priori the right closures and the right boundaries between spherical and deformed nuclei, we now that extremely good fits can be obtained with monopole-like forms [10].

Let us see how in the present formulation $H_M$ is expected to provide naturally good boundaries, once $H_m$ has provided good closures. The second part of Table 1 lists the four possible operators whose appearance is guaranteed under very general circumstances for spherical nuclei. To a large extent they account for subshell effects. They are discussed in detail in [5]. The $D^b$ factors reflect scaling uncertainties to be resolved by the fit.

Nilsson diagrams indicate that the onset of deformation is associated with the interruption of normal spherical filling by the promotion of 4 neutrons and 4 protons to configurations in the next HO shell (i.e. including the $j$ orbit as well as others) [5]. Calling $q_i$ the quadrupole moment of these intruders and $q$ that of the orbits left behind, we expect a gain in energy of the form

$$(q + q_i)^2 = q^2 + q_i^2 + 2qq_i$$

. In the third part of Table 1 we give the expressions for $QQ0$ and $QQ1$ representing the two possible $q^2$ contributions. Since $q_i$ is a constant, its effects are included in the DK term meant to correct the estimate of monopole loss coming from $H_m$. The $qq_i$ terms are conceptually important since $q_i$ provides the effective quadrupole strength that will drive the lower orbits. However, we have left them out of the table because the information and the few keV they bring do not justify bothering with 4 extra parameters. Conversely $JU$ is introduced explicitly to stress that by varying it, $JU = 4$ turns out to be optimal. The form of $q$ is equivalent to equidistant Nilsson orbits and it is scaled so that deformation energies have a standard $A^{1/3}$ behaviour.

All operators (except $V_c$) are affected by factors of type (8) with $\xi = 0.42$ in $R_c$. Energies (taken to be positive) are given by the expectation values

$$E(N, Z) = <H_m> + <H_s>(1 - \delta_d) + <H_d> \delta_d$$

$$= \max(<H_m> + <H_s>, <H_m> + <H_d>) \quad (11)$$

the lowest possible orbits are filled for spherical nuclei ($\delta d = 0$), while for deformed ones ($\delta d = 1$), $JU \cdot \rho$ particles are promoted to orbits $j$. The calculations are conducted

| Table II. Parameters of the 14p, 28p, 28p$^*$ and 20p fits. ($V_p$ and $V_c$ given in Table 3). 28p$^*$ fit uses $R = A^{1/3}$. |
|---------|---|---|---|---|---|---|---|---|---|---|
| $\Gamma$ | $F M^+$ | $P M^+$ | $4T(T+1)$ | $F S^+$ | $F C^+$ | $S 3$ | $D K$ | $Q Q^-$ | $P S^+$ | $P S^-$ |
| $\rho(\Gamma)14$ | 9.33 | -0.602 | -36.08 | 0.44 | 3.27 | 0.45 | -10.0 | 6.53 |
| $\rho(\Gamma)28$ | 9.51 | -0.79 | -36.51 | 5.19 | -15.15 | 0.56 | -36.1 | 21.6 | -0.7 | -0.1 | 1.0 | -30.01 | 0.4 | 3.6 |
| $\rho(\Gamma)28^*$ | 9.55 | -0.82 | -31.83 | 5.26 | -26.75 | 0.57 | -36.9 | 19.0 | -0.7 | -0.1 | 1.05 | -26.75 | 0.4 | 2.6 |
| $\rho(\Gamma)20$ | 9.67 | -0.95 | -34.77 | 5.95 | -20.73 | 0.54 | -44.2 | 27.5 | -0.7 | -0.16 | 1.07 | -20.73 | 0.4 | - |

by initializing $\delta d$, fitting $E(N, Z)$ in the first equality of eq.(11) to the 1751 mass values for $N, Z \geq 8$ in the latest compilation [10], then resetting $\delta d$ through the second part of eq.(11) and iterating until convergence. Table 2 contains results for 3 fits with 14, 28 and 20 parameters (14p, 28p, 20p), whose RMS errors are 614, 388 and 423 KeV respectively. The notation for the operators is 

$\hat{\Gamma} FM + PM + 4T(T + 1) \quad FS + FC + S_3 \quad DK \quad QQ^- \quad PS + PS^- \quad FS^- \quad FC^- \quad SQ^- \quad QQ^+$

In 28p, we have added two $QQ^+$ and two $SQ^-$ parameters for a gain of 60 keV, and 10 parameters associated with spin orbit effects that bring in 150 keV. With 28 parameters, Table 2 and 3 compare the $\xi = 0.42$ (28p) and $\xi = 0$ (28p$^*$) choices for $R_c$.

The 20p fit is a variation of 28p in which $QQ^+$ is excluded and five groups of operators: ($F M^+, P M^+$), ($4T(T + 1)$), ($QQ^-$), ($F S^+, F C^+$), ($P S^+, D K, S Q^-$) are constrained to have a single $\rho(\Gamma)$ per group.
TABLE III. Asymptotic forms of the fits compared with a pure LD form $(6p)$. $(T2$ is for $4T(T+1))$

|   | $A$     | $-A^{2/3}$ | $-T2/A$ | $T2/A^{4/3}$ | $V_c$  | $V_{rc}$ | RMS |
|---|---------|------------|---------|--------------|--------|----------|-----|
|6p | 15.49   | 17.79      | 28.64   | 40.23        | 5.22   | 0.705    | 2.544 |
|14p| 14.95   | 12.43      | 26.73   | 36.21        | 5.17   | 0.696    | 0.614 |
|28p| 14.95   | 12.14      | 27.26   | 37.51        | 5.21   | 0.699    | 0.388 |
|28p*|14.98    | 12.21      | 28.50   | 40.66        | 5.25   | 0.699    | 0.409 |
|20p| 14.99   | 12.36      | 27.24   | 37.30        | 5.21   | 0.699    | 0.423 |

Subshell effects. The $H_\alpha$ operators are largely devoted to mock the energy patterns generated by subshell structure [3]. The $S2$ operator is easily absorbed in $H_m$ and the heaviest task goes to $S3$. Parametrization (8) is now a convenient tool unrelated to its original derivation (eqs.(6) and (7)). This can be detected by an anomalously large $\rho$ value leading to a change in sign of $S3$ at $R = \rho$, i.e. $A \geq 100$, the region in which $j$ orbits can start filling before $r$ orbits are full. In general, a large $\rho(\Gamma)$ indicates that the $\Gamma$ operator is adding to its specific job some subshell corrections (e.g. $\rho(QQ^-)$ in $28p$, for a gain of 25 keV, and $\rho(DK)$ ($= \rho(S3)$!) for a gain of 100 keV already mentioned). Given that SO is the very origin of subshell structure it comes as no surprise that $S$-type operators are easily contaminated by large $\rho$ ratios.

LD parameters and radii. Table 3 compares the parameters of $6p$ (pure LD) with those obtained by expanding eq.(5) and similar ones for $FM$ and $PM+$: the combinations $1.717[(FM+) + (PM+)]$ and $4T(T+1) + (0.382 + 1.145c)([FM+] + (PM+)]$

become the asymptotic coefficients of $A$ and $4T^2$ respectively. The factor in $\xi$ comes from the $R$ denominators. It doubles for the $4T^2/A^{4/3}$ term. The gain brought about by the use of a more precise form of $R_c$ is no doubt significant as shown by the case of $28p$.

It should be noted that with $\alpha = 1/2$ scaling, $PM+$ is a volume term, while for $\alpha = 0$ it is pure surface and $\rho(FM+)$ becomes very small, a disturbing result that justifies the $\alpha = 1/2$ choice.

It is remarkable, also, that the radius extracted for $V_c$ in Table 3, $r \approx 1.235 R_c$, is very close to the fitted $r \approx 1.225 R_c$

The $FMT - 4T(T + 1)$ puzzle. The presence of the $4T(T+1)$ term is demanded by the fits below 650 keV, while the omission of $FMT$ is possible down to the 470 keV level. The puzzle is that it serves no purpose to treat $FMT$ as a free parameter: the efficient combination is $FM+ = FMA + FMT$. Renormalisation effects and the cancellation of kinetic and potential energies are the only guesses we can propose for the emergence of $T(T+1)$ and $FMA + FMT$ as leading operators.

Deformed nuclei. To avoid unphysical results we allow $\delta d = 1$ in eq.(11) only when $DK > 0$, i.e. for $A \geq 100$. The number of $\delta = 1$ cases is $(423, 367, 329)$ for the $(14p, 28p, 20p)$ fits, and the RMS errors of $(594, 302, 385)$ are smaller than those for the spherical nuclei in each case. The experimental ground state bands of the $\delta d = 1$ nuclei show rotational features.

To conclude: by replacing the global-local alternative by the monopole-multipole separation of $H$ we can find good mass formulae. Better ones will come once we learn more about $H_m$.

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[1] ADNDT 39, 2 (1988) (P.E. Haustein Special Editor)
[2] S. Liran and N. Zeldes, ADNDT 17 (1976), 431
[3] J.M. Pearson, Y. Aboussir, A.K. Dutta, R.C. Nayak, and M. Farine, Nucl. Phys. A528 (1991), 1
[4] P. Möller, J.R. Nix, W.D.Myers and W.J. Swiatecki, submitted to ADNDT (1993)
[5] A.P. Zuker, Nucl. Phys. (1994) (to be published)
[6] M. Dufour and A.P.Zuker, CRN 93-29 (1993)
[7] A. Abzouzi, E. Caurier and A.P. Zuker, PRL 66 (1991), 1134
[8] A. Bohr and B. Mottelson, Nuclear Structure I (Benjamin, New York, 1964)
[9] J. Duflo *Nucl. Physics* (1994) (to be published)
[10] G. Audi and A.H. Wapstra *Nucl. Physics A565* (1993), 1