Semiempirical Shell Model Masses with Magic Number $Z = 126$ for Translead Elements with $N \leq 126$

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A semiempirical shell model mass equation based on magic number $Z = 126$ and applicable to translead elements with $N \leq 126$ is presented. For $\alpha$-decay energies the equation is shown to have a high predictive power and an rms deviation from the data of about 100 keV. The rms deviations for masses and other mass differences are between about 200 and 300 keV.

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Recent progress in superheavy elements (SHE) research reaching to $^{293}118$ and its $\alpha$-decay products [1] makes it necessary to find an appropriate substitute for the semiempirical shell-model mass equation (SSME) [2] (see also ref. [3]) for nuclei in the neighbourhood of $Z = 114$ and beyond [4]. The $\alpha$ energies of the decaying chain vary smoothly from $^{293}118$ to $^{269}\text{Sg} (Z = 106)$, with no indication of magicity at $Z = 114$ in these nuclei [4], whereas the SSME assumes that $Z = 114$ is the next spherical proton magic number after lead and it stops there. Furthermore, the SSME becomes unsuitable for extrapolation already earlier, beyond Hs ($Z = 108$), as shown by its increasing deviations from the data when $Z$ increases. (Like in fig. 4 of ref. [1].)

Recent phenomenological studies of BE(2) systematics [5] and of the persistence of the Wigner term in masses of heavy nuclei [6] indicate $Z = 126$ as the next spherical proton magic number after lead, and this is consistent with considerations based on nuclear diffuseness [7]. Recent self-consistent and relativistic mean-field calculations [8–12] variously predict proton magicities for $Z = 114, 120, 124$ and 126.

During the early stages of the SSME [13], when it was adjusted separately in individual shell regions in the $N - Z$ plane, both $Z = 114$ and $Z = 126$, which were at the time considered possible candidates for the postlead proton magic number (see, e.g., ref. [14]), were tried as a shell region boundary in each of the two heaviest regions with $Z \geq 82$ and respective $N$-boundaries $82 \leq N \leq 126$ (called here region A) and $126 \leq N \leq 184$ (called region B). The agreement with the data was about the same for both choices, and the prevailing view in the mid nineteen-seventies led to the choice of $Z = 114$ for the SSME mass table [3]. In a recent communication [4] we showed that the early $Z = 126$ results have a high predictive power in the interior of region B and proposed their use there as a predictive tool in SHE research. In the present note we study the predictive power or

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extrapolatability of the early $Z = 126$ results in region A and propose a mass equation based on them as a substitute for the SSME [2] in the interior of the region. The study is based on the newer data that became available after the adjustments were made, as was done in refs. [4, 15–18].

In the SSME the total nuclear energy $E$ is a sum of pairing, deformation and Coulomb energies:

\[ E(N, Z) = E_{\text{pair}}(N, Z) + E_{\text{def}}(N, Z) + E_{\text{Coul}}(N, Z). \]  

The form of $E_{\text{Coul}}$ is the same in all shell regions:

\[ E_{\text{Coul}}(N, Z) = \left( \frac{2Z_0}{A} \right)^{1/3} \left[ \alpha^c + \beta^c (Z - Z_0) + \gamma^c (Z - Z_0)^2 \right], \]  

and that of $E_{\text{pair}}$ is the same separately in all diagonal shell regions, where the major valence shells are the same for neutrons and for protons, and in all non-diagonal regions, where the neutron and proton valence shells are different. Unlike in [2], with $Z = 126$ rather than 114 as an upper proton boundary, region A becomes a diagonal region with

\[ E_{\text{pair}}(N, Z) = \left( \frac{A_0}{A} \right) \left[ \alpha + \beta (A - A_0) + \gamma (A - A_0)^2 + \varepsilon T (T + 1) + \frac{1 - (-1)^A}{2} \Theta + \frac{1 - (-1)^{NZ}}{2} \kappa \right], \]  

The part $E_{\text{def}}$ for region A with $Z = 126$ as upper proton boundary is

\[ E_{\text{def}}(N, Z) = \left( \frac{A_0}{A} \right) \left[ \phi_{11} \Phi_{11}(N, Z) + \psi_{20} \left[ \Psi_{20}(N, Z) + \Psi_{20}(Z, N) \right] \right] \]  

with

\[ \Phi_{11}(N, Z) = (N - 82) (126 - N) (Z - 82) (126 - Z) \]  

and

\[ \Psi_{20}(N, Z) = (N - 82)^2 (126 - N)^2 (N - 104). \]

In eqs. (2)–(4) $A = N + Z$ and $T = |T_z| = \frac{1}{2}|N - Z|$. The respective values of $Z_0$ and $A_0$ are 82 and 164. The coefficients multiplying the functions of $N$ and $Z$ are adjustable parameters which were determined by a least-squares adjustment to the data [13]. Their numerical values resulting from that adjustment are given in the second column of table I. The mass excesses $\Delta M(N, Z)$ are obtained by adding to eq. (1) the sum of nucleon mass excesses $N \Delta M_n + Z \Delta M_H$.

The experimental data used in the adjustment included 29 masses and 62 $Q_\alpha$ values connecting unknown masses (Ref. [20] augmented by data from the literature up to Spring 1973). Presently there are 150 known experimental masses in region A and 3 $Q_\alpha$ values

\[ \text{In the as yet unknown odd-odd } N = Z \text{ translead nuclei the g.s. is expected to have } T = |T_z| + 1 \text{ and seniority zero, whereas eq. (1) with } T = |T_z| \text{ gives the energy of a low excited seniority two state [3]. (See also ref. [19].)} \]
connecting unknown masses (Refs. [21] (excluding values denoted “systematics” (#)) and [22], augmented by data from the recent literature). There are 121 new masses that were not used in the adjustments.

Fig. 1 shows the deviations from the data of the predictions of eq. (1) (with the definitions (2)−(4) and the coefficients from the second column of table I) for all the 150 known masses. The deviations are plotted as function of the distance from the line of β-stability, denoted “neutrons from stability” (NFS) and defined by \( NFS = N - Z - \frac{0.44A^2}{A+200} \). Empty circles denote the deviations of the 29 originally adjusted masses and full circles mark the deviations of the 121 new masses. The original deviations are relatively small. The new deviations are mostly considerably larger and are almost all negative. There is a large scatter of the points, superposed on an overall decreasing trend when NFS increases in the negative direction. For closer scrutiny we show in fig. 2 lines connecting deviations of Pb, Bi, Po and At isotopes as function of \( T \) rather than NFS. Isotopic lines of other elements follow closely. There is an odd-even staggering of the points, where for even-even and odd-odd nuclei the deviations are respectively higher and lower than for odd-mass ones, and there is an overall increasing overbinding when \( T \) decreases away from stability. The increasing staggering when \( T \) decreases as compared to the old data indicates increasing pairing parameters Θ (see also ref. [23]) and (even more so) \( \kappa \) towards the proton drip line. Similarly, the increasing binding when \( T \) decreases indicates that the symmetry-energy parameter \( \varepsilon \) decreases towards the drip line.

Table II, patterned after similar more elaborate ones [16,17] (see also ref. [4]), shows the values of \( \delta_{av} \) and \( \delta_{rms} \), the respective average and rms deviations of eq. (1) from the data, for \( \Delta M, S_n, S_p, Q_{\beta^-} \) and \( Q_{\alpha} \). The deviations are shown separately for the older data that were used in the adjustment and for the newer data. The last column shows the error ratios \( \delta_{rms}^{new} / \delta_{rms}^{old} \).

For the older data the \( \delta_{av} \) are few tens keV at most, and the \( \delta_{rms} \) are in the range 100-250 keV. For the newer nuclei the agreement with the data of predicted \( \Delta M \) (fig. 1), \( S_n, S_p \) and \( Q_{\beta^-} \) values has much deteriorated. On the other hand, the \( \delta_{rms} \) of the predicted \( Q_{\alpha} \) values has even very slightly improved. The \( Q_{\alpha} \) deviations, both old and new, are remarkably small.

The high degree of extrapolatability of the \( Q_{\alpha} \) values as compared to the poorer predictions of \( \Delta M, S_n, S_p \) and \( Q_{\beta^-} \) is presumably due to the composition of the old data set used in the adjustments. The coefficients \( \beta, \gamma, \beta^c, \gamma^c, \varphi_{11} \) and \( \psi_{20} \), which contribute to both mass and \( Q_{\alpha} \) values, and also \( \alpha^c \), which was determined using \( \beta^c \) and \( \gamma^c \) [13] (see also ref. [24]), were determined by all the 91 available mass and \( Q_{\alpha} \) data. On the other hand, neglecting their \( A \)-dependence the coefficients \( \alpha, \varepsilon, \Theta \) and \( \kappa \) cancel in \( Q_{\alpha} \) and they were determined essentially by the smaller group of 29 masses found in the nearest-to-stability corner of the shell region, with too-small values of \( \Theta \) and \( \kappa \) and too large value of \( \varepsilon \) as compared to more proton-rich nuclei. These values, which to a large extent cancel in \( Q_{\alpha} \), are responsible for the large deviations of the predicted new masses.

One would like to restore to the new \( \Delta M, S_n, S_p \) and \( Q_{\beta^-} \) predictions the same degree of agreement with the data as the old predictions had, while at the same time retaining the high quality of \( Q_{\alpha} \) predictions. For eq. (1) this goal might most simply be approached by making a least-squares adjustment of eq. (1) to all the 150 known masses, with only four adjustable parameters \( \alpha, \varepsilon, \Theta \) and \( \kappa \), while the other seven coefficients are held fixed.
on their old values from the second column of table I. The re-adjusted parameters $\alpha$ and $\varepsilon$ would correct the systematic overbinding when $T$ decreases, and the re-adjusted $\Theta$ and $\kappa$ would decrease the odd-even staggering of the deviations.

The re-adjusted values of the coefficients $\alpha, \varepsilon, \Theta$ and $\kappa$ are given in the third column of table I. Their changes compared to the second column are in the anticipated directions. The respective average and rms mass deviations obtained in the adjustment for all the 150 mass data are 2 and 246 keV.

Fig. 3 shows the deviations from the data of the predicted mass values resulting from the new adjustment, similarly to fig. 1. For ease of comparison the same nuclei are denoted by the same kind of circle (empty or full) in the two figures. The deviations for the post 1973 measured nuclei (denoted by full circles) and their odd-even staggering are considerably smaller than in fig. 1, and the overall decreasing trend when $T$ decreases has largely disappeared, as was expected. The deviations for the older data have worsened, though, and there is a new overall oscillatory trend not observed in fig. 1, indicating that enlarging eq. (1) by additional particle-hole symmetric $E_{\text{def}}$ terms (eq. (4)) might reduce the deviations further.

Table III shows the resulting $\delta_{av}$ and $\delta_{rms}$ values of the predicted deviations. Like in table II they are shown separately for the old 1973 data nearer to stability and for the new data extending into the interior of region A towards the proton drip line. For $S_n, S_p$ and $Q_\alpha$ the new deviations are similar to those of the original nuclei in table II. For $\Delta M$ and $Q_\beta$– the $\delta_{rms}$ are respectively 1.5 and 1.1 times larger.

The new mass deviations shown in table III are about one half to two thirds of the corresponding deviations of several recent mass models [16, 17, 25, 26], and for $Q_\alpha$ they are smaller. The smaller values of the deviations in table III are presumably due mainly to the inclusion of the particle-hole symmetric configuration-interaction terms $E_{\text{def}}$ (eq. (4)) in eq. (1). Until a new adjustment of the $Z = 126$ SSME to the data in both regions A and B is undertaken, which would further reduce the deviations in both regions, we propose the use of eq. (1), with the new values of $\alpha, \varepsilon, \Theta$ and $\kappa$ and the old values of the other coefficients, given in table I, as a predictive tool for masses and their differences, and particularly for the extrapolatable-proven $Q_\alpha$ values, in the interior of region A.

It should be emphasized, though, that the above results are not a proof of superior magicity of $Z = 126$ in region A as compared to other recently proposed prediction [11, 12], because no comparative studies of this kind were made. (See also ref. [14].)

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Table 1
Values of the coefficients of eq. (1) as determined by adjustment to the old data [13] (Old Value) and as readjusted in the present work (New Value).

| coefficient | Old Value (keV) | New Value (keV) |
|-------------|-----------------|-----------------|
| $\alpha$    | $-1.9902575 \times 10^6$ | $-1.987628 \times 10^6$ |
| $\beta$     | $-2.4773664 \times 10^4$ | $-2.487628 \times 10^4$ |
| $\gamma$    | $-8.51085 \times 10^1$   | $-8.51085 \times 10^1$   |
| $\varepsilon$ | $4.658516 \times 10^2$   | $4.585496 \times 10^2$   |
| $\Theta$    | $9.762 \times 10^2$      | $1.2183 \times 10^3$     |
| $\kappa$    | $1.4965 \times 10^3$     | $2.1937 \times 10^3$     |
| $\alpha^c$  | $7.968418 \times 10^5$   | $7.968418 \times 10^5$   |
| $\beta^c$   | $2.032906 \times 10^4$   | $2.032906 \times 10^4$   |
| $\gamma^c$  | $9.819137 \times 10^1$   | $9.819137 \times 10^1$   |
| $\varphi_{11}$ | $-4.794 \times 10^{-2}$ | $-4.794 \times 10^{-2}$ |
| $\psi_{20}$ | $9.095 \times 10^{-4}$   | $9.095 \times 10^{-4}$   |

Table 2
Numbers of data N, average deviations $\delta_{av}$, and rms deviations $\delta_{rms}$, for eq. (1) with the old values of the coefficients from Table I. The last column shows the error ratios $\delta_{rms}^{new}/\delta_{rms}^{old}$.

| Data          | $\delta_{av}$ (keV) | $\delta_{rms}$ (keV) | $\delta_{av}$ (keV) | $\delta_{rms}$ (keV) | Error ratio |
|---------------|---------------------|----------------------|---------------------|----------------------|-------------|
| $\Delta M$    | 29                  | $-29$                | 146                 | $-807$               | 1008        | 6.88        |
| $S_n$         | 18                  | 39                   | 214                 | $-120$               | 406         | 1.90        |
| $S_p$         | 22                  | 9                    | 182                 | 104                  | 132         | 2.29        |
| $Q_{\beta^-}$ | 15                  | $-20$                | 242                 | 101                  | 248         | 2.41        |
| $Q_\alpha$    | 78                  | 5                    | 103                 | 31                   | 40          | 0.87        |

Table 3
Numbers of data N, average deviations $\delta_{av}$, and rms deviations $\delta_{rms}$, for eq. (1) with the new values of the coefficients $\alpha, \varepsilon, \Theta, \kappa$ and the old values of the other seven coefficients from Table I.

| Data          | $\delta_{av}$ (keV) | $\delta_{rms}$ (keV) | $\delta_{av}$ (keV) | $\delta_{rms}$ (keV) |
|---------------|---------------------|----------------------|---------------------|----------------------|
| $\Delta M$    | 29                  | $-193$               | 344                 | 121                  | 48          | 216        |
| $S_n$         | 18                  | 158                  | 416                 | 120                  | $-10$       | 205        |
| $S_p$         | 22                  | $-144$               | 202                 | 104                  | 18          | 184        |
| $Q_{\beta^-}$ | 15                  | $-257$               | 475                 | 101                  | 15          | 277        |
| $Q_\alpha$    | 78                  | $-5$                 | 104                 | 31                   | 18          | 85         |
Figure 1. Deviations of the predicted masses [13] from the presently known data in region A. Shown as function of Neutrons From Stability (NFS).

Figure 2. Isotopic lines of predicted mass deviations [13] of Pb, Bi, Po and At nuclei measured after the adjustments were made. Shown as function of $T$. 
Figure 3. Deviations of the predicted masses resulting from the present adjustment from the presently known data in region A. Shown as function of NFS.