New effective Hamiltonians for the sd shell

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Abstract. We derive new Hamiltonians for the sd-shell, USDA and USDB, based on a renormalized G matrix with linear combinations of two-body matrix elements adjusted to fit a complete set of data for experimental binding energies and excitation energies for the sd-shell nuclei. These Hamiltonians provide a new level of precision for realistic sd-shell wavefunctions for applications to nuclear structure and nuclear astrophysics.

The USD Hamiltonian \cite{1, 2} has provided realistic sd-shell \((0d_5/2, 0d_3/2, 1s_1/2)\) wavefunctions for use in nuclear structure models, nuclear spectroscopy and nuclear astrophysics for over two decades. The original USD Hamiltonian was obtained from a least square fit of 452 energy data with experimental errors of 0.2 MeV or less (most experimental errors are 10 keV or less) from 66 nuclei. The root-mean-square (rms) deviation between experimental and theoretical energies was about 150 keV. Although many energy levels were known in the middle of the shell only a few were included in the USD fit due to the computational limitations in the 1980. Also since 1980 there is much more and improved data for the neutron-rich nuclei. Today the computational effort is trivial - on a desktop PC it is possible to obtain a complete set of low-lying energy levels for all sd-shell nuclei in a few hours. Thus we are motivated to refine the derivation of the USD Hamiltonian with an updated and complete set of energy data. We are able to consider 608 states in 77 nuclei. The new Hamiltonians USDA and USDB lead to a new level of precision for realistic shell-model wavefunctions.

The data for the new fits was obtained from the most recent compilations. In the case of \(A = 21-40\) nuclei most data for excited states are from the Supplement to Energy Levels of \(A = 21-44\) nuclei by P. M. Endt (published in 1998 \cite{3}), used in conjunction with the previous complete review of nuclei in this mass range \cite{4}. More recent data is taken from: \(^{20}\text{O} \cite{5, 6}, ^{21}\text{O} \cite{6}, ^{23}\text{O} \cite{7, 22}\text{O} \cite{6}, ^{19}\text{F} \text{and} ^{20}\text{F} \cite{8}, ^{22}\text{F} \cite{8, 9}, ^{23}\text{F} \text{and} ^{25}\text{F} \cite{10, 27}\text{F} \cite{11}, ^{24}\text{Ne} \cite{12, 27}\text{Na} \cite{13}, ^{28}\text{Na} \text{and} ^{29}\text{Na} \cite{14}, ^{24}\text{Mg} \cite{15} \text{and} ^{33}\text{Si} \cite{16}. The ground-state binding energies used are from the 2003 atomic mass evaluation of Audi, Wapstra and Thibault \cite{17}. These are supplemented with new results from Ref. \cite{18} for \(^{23}\text{O}, ^{23}\text{F}, ^{24}\text{O}, ^{25}\text{F}, ^{26}\text{F}, ^{27}\text{F}, ^{27}\text{Ne}, ^{28}\text{Ne}, ^{29}\text{Ne}, ^{30}\text{Ne}, ^{31}\text{Na} \text{and} ^{32}\text{Mg}.\" We take the binding energies relative to that of \(^{16}\text{O}\) with the Coulomb energy correction used for USD \cite{19} \(BE(A, Z)^r = BE(A, Z) - BE(^{16}\text{O}) - EC(Z)\) with \(EC(Z) = 3.48 (Z=9), 7.45 (Z=10), 11.73 (Z=11), 16.47 (Z=12), 21.48 (Z=13), 26.78 (Z=14), 32.47 (Z=15), 38.46 (Z=16), 44.74 (Z=17), 51.31 (Z=18) \text{and} 58.14 (Z=19)\) MeV. The Coulomb energy corrections were obtained from energy differences of isobaric analogue states for the nuclei near \(N=Z\).
The shell-model effective Hamiltonian can be written as sum of one- and two-body operators:

\[ H = \sum_a \epsilon_a \hat{n}_a + \sum_{a \leq b, c \leq d} \sum_{J^T} V_{JT}(ab;cd) \hat{T}_{JT}(ab;cd), \]

where \( \hat{n}_a \) is the number operator for the spherical orbit \( a \) with quantum numbers \( (n_a, l_a, j_a) \), and

\[ \hat{T}_{JT}(ab;cd) = \sum_{MT_z} A_{JMT_z}^l(ab) A_{JMT_z}^T(cd) \]

is the scalar two-body density operator for nucleon-pairs in orbits \( a, b \) and \( c, d \) coupled to spin quantum numbers \( JM \) and isospin quantum numbers \( TT_z \). We use a simplified notation

\[ H = \sum_{i=1}^p x_i O_i, \]

where the \( x_i \) stand for single-particle energies \( \epsilon_a \) or the two-body matrix elements \( V_{JT}(ab;cd) \), and the operators \( O_i \) stand for \( \hat{n} \) or \( \hat{T} \), respectively. The vector \( \vec{x} = (x_1, x_2, \cdots, x_p) \) defines the Hamiltonian. This Hamiltonian will have eigenvectors \( \phi_k \) and eigenvalues \( \lambda_k \) that can be expressed in terms of a linear combination of the Hamiltonian \( \vec{x} \)

\[ \lambda_k = \langle \phi_k | H | \phi_k \rangle = \sum_{i=1}^p x_i \langle \phi_k | O_i | \phi_k \rangle = \sum_{i=1}^p x_i \beta_k^i, \]

where \( \beta_k^i = \langle \phi_k | O_i | \phi_k \rangle \).

For a given starting Hamiltonian \( \vec{x}^s \), we calculate \( \beta_k^i \) and then minimize the quantity

\[ \chi^2 = \sum_{k=1}^N \left( \frac{E_{\text{exp}}^k - \lambda_k}{\sigma_{\text{exp}}^k} \right)^2, \]

where \( E_{\text{exp}}^k \) are the experimental energies, and \( \sigma_{\text{exp}}^k \) are the associated errors. Thus we obtain an improved Hamiltonian \( \vec{x} \). To take into account the implicit dependence of \( \beta_k^i \) on \( x_j \) this procedure is repeated (iterated) until convergence.

As in most multi-parameter fits, the resulting parameters \( x_i \) are highly correlated. In addition, the low-lying nuclear states are much more sensitive to some linear combinations of Hamiltonian parameters than others. It is possible to reformulate the fit in terms of uncorrelated linear combinations. The orthogonal parameters \( y_i \) are linear combinations of the Hamiltonian parameters \( x_i \), with associated errors \( d_i \). We can separate poorly determined linear combinations from well-determined ones by setting a certain criterion on the magnitude of the corresponding eigenvalues \( d_i \). The poorly determined linear combinations of Hamiltonian parameters were always constrained to the values obtained from the renormalized \( G \) matrix applied to the sd shell (RGSD), based on the Bonn-A \( NN \) potential. The TBME are given in Table 20 of [20]. The calculations for the wavefunctions, energies, occupation numbers and scalar two-body transition densities were carried out with Oxbash [21]. One iteration took about 12 hours on a desktop PC.

For the data set we consider all ground-state binding energies and all positive-parity energy levels for sd-shell nuclei. The first criterion for inclusion of the \( n \)th \( J^\pi \) level in the fit is whether or not the \( J^\pi \) for all lower states are known. Generally this means that we cannot consider states above the energy where one level has an unknown \( J^\pi \). This usually occurs starting at \( E_x = 5-7 \text{ MeV} \). The second criterion is the energy at which the experimental level density for a given \( J^\pi \) becomes suddenly higher than the theoretical level density. This is a signature of...
intruder states. There is a well-defined region of nuclei with $N = 19 - 20$ and $Z = 10 - 12$ where the difference between the experimental and theoretical ground-state binding energies is much larger that the rms average. These nuclei are in the island-of-inversion that requires the explicit extension of the $pf$ shell orbits to the model space [22]. Ground and excited states for these six nuclei are not included in the fit.

With this selection we are able to consider 608 states in 77 nuclei with errors of less than 0.2 MeV (most experimental errors are 10 keV or less). The uncertainty used in Eq. (5) is the experimental uncertainty $\sigma_{exp}$ folded quadratically with a theoretical error that is close to the rms value obtained in the best fit for which we take $\sigma_{th} = 0.1$ MeV; $(\sigma_{k})^2 = (\sigma^{k}_{exp})^2 + (\sigma^{k}_{th})^2$. As was done for USD, we employ a mass dependence of the two-body matrix elements of the form

$$V_{JT}(ab; cd)(A) = \left( \frac{18}{A} \right)^p V_{JT}(ab; cd)(A = 18),$$

with $p = 0.3$. This accounts qualitatively for the mass dependence expected from the evaluation of a medium-range interaction with harmonic-oscillator radial wavefunctions.

For the present work the original USD Hamiltonian was used for the first iteration. Then the equations were iterated with $N_d = 30$ well-determined (varied) linear combinations with the remaining 36 poorly-determined linear combinations set to the RGSD values. This was continued until the energies and $\vec{x}$ values converged to the level of about 10 keV. This rather highly constrained Hamiltonian is called USDA. The rms deviation between experimental and theoretical energies is given by

$$rms = \sqrt{\frac{\sum_{k=1}^{N} (E_{exp}^k - E_{th}^k)^2}{N}}.$$  

(7)

In Fig. (1) we show this rms deviation (solid line) as a function of the number of varied linear combinations $N_d$ obtained for the final iteration of USDA (the actual USDA corresponds to the results obtained at $N_d = 30$). The rms deviation of the fitted and RGSD two-body matrix elements as a function of $N_d$ are shown by the points connected by a dashed line in Fig. (1).

The motivation for 30 linear combinations can be seen in Fig. (1). One observes a plateau in the rms energy deviation of about 170 keV between 30 and 45 linear combinations. Beyond this there is a gradual drop until about 56 linear combinations with an rms deviation of 130 keV that does not significantly decrease going out to the full set of 66 combinations. Thus we also derive another Hamiltonian called USDB by varying 56 linear combinations of parameters. The individual contributions to Eq. (7) are given Fig. (2) for USDB. We include in the two figures six data points not included in the fit, i.e. those for the ground states of $^{29,30}$Ne, $^{30,31}$Na, and $^{31,32}$Mg to show the large deviations for these nuclei in the island of inversion.

Thus we have two new Hamiltonians, a conservative one, USDA, closest to RGSD that gives a good but not the best fit to data, and another, USDB, that differs more from RGSD but gives an best fit to data. Calculation of other observables such as spectroscopic factors, moments, gamma decay and beta decay rates with both USDA and USDB will give an estimate of the theoretical errors due to the sd-shell Hamiltonian as well as determine whether or not USDB is in fact superior to USDA.

For the binding energies, is it instructive to compare the results of the original USD with the updated set of data. The USD binding energies are given in Fig. (3). Most of the differences lie in the nominal rms range of 150 keV. The binding energies predicted for the neutron-rich fluorine ($Z=9$) isotopes turn out to be larger than experiment by up to 1.5 MeV. This indicates that the USD TBME involving the $d_{3/2}$ orbital in this mass region are incorrect. The oxygen isotopes ($Z=8$) beyond $N=16$ are known to be unbound [23], [24], [25], [26], [27], [28] and the neutron decay properties are not yet measured. The USD predicts that these nuclei are unbound except...
Figure 1. Rms deviations as a function of the number of fitted linear combinations. The points connected by a line shows the deviation between experimental and theoretical sd-shell energies. The points connected by a dashed line shows the rms deviation between the two-body matrix elements for the fitted and RGSD Hamiltonians.

Figure 2. Deviations between experimental and theoretical energies for USDB. The ground state binding energies are plotted in the top and the excitation energies in the bottom. The inset shows a histogram of the deviations binned over 100 keV intervals.

For $^{26}$O which is bound by 1.0 MeV with USD. Thus both neutron-rich oxygen and fluorine are too tightly bound with USD. In contrast the binding energies predicted for $Z=10$-$12$ and $N=20$ are larger than experiment by up to 1.5 MeV. This indicates that the USD TBME are incorrect or that other shell-model configurations dominate the wavefunctions.

The fluorine problem for USD is corrected by the new USDA and USDB Hamiltonians. The results for USDB are shown in Fig. (4). In addition all of the oxygen isotopes with $N \geq 16$ are are unbound with USDA and USDB. However, the $Z=10$-$12$, $N=20$ difference cannot be corrected, confirming the intruder state (island-of-inversion) interpretation for these nuclei. The improved USDA and USDB results for the ground state binding energies of the neutron-rich fluorine and oxygen isotopes are related to the increased energy for the effective $d_{3/2}$ SPE. We note that this particular problem with USD was corrected when it was applied to the $sd-pf$ model space [29].

Spectra were calculated for all 87 sd-shell nuclei for both USDA and USDB and compared to experiment. The compete set of comparisons can be found on the web [30]. As an example, we show the results for $^{26}$Al and $^{26}$Mg in Figures (5) and (6), respectively. Experiment is shown on the left-hand side with lines that indicate the $J$ value for the known positive-parity states. The lowest $J$ value is labeled. Levels with an unknown $J^\pi$ assignment are shown by the shortest lines, with the first such level for $^{26}$Al lying at about 4 MeV. The theoretical levels are shown on the right-hand side, also indicated by lines of different length for the $J$ value. The experimental and theoretical levels joined by a line in the middle are those included in the fit. The slope of these lines shows the difference between experiment and theory for the excitation energy.
The ground state binding energies are shown at the bottom. Starting at about 4 MeV we cannot make a level to level assignment between theory and experiment due to the incomplete experimental information. From 4-6 MeV the experimental and theoretical level densities are similar; but there are too many levels of unknown spin-parity to make definitive associations between experiment and theory.

Above 6 MeV in $^{26}$Al the experimental level density becomes higher, indicating the onset of intruder states, e.g. wavefunctions that contain the excitation of two or more nucleons out of the 0p shell or into the 1p0f shell. Generally toward the beginning and end of the sd-shell where the sd-shell level density is smaller, the intruder states are more obvious in the low-lying spectra.
For example in $^{18}$O two 0$^+$ states appear below 6 MeV compared to only one in the theory. The structure of this extra 0$^+$ in terms of p-shell excitations is well known [31]. In the upper part of the sd-shell we find for example the lowest 2$^+$ state in $^{34}$Si experimentally at 3.2 MeV and theoretically at 5.2 MeV. The lowest 2$^+$ state is interpreted as the neutron 2$p - 2h$ configuration that becomes the ground state in the island-of-inversion nuclei $^{32}$Mg and $^{30}$Ne [29].

The systematic application of USDA and USDB to other observables such as moments, electromagnetic decay and beta decay will be carried out over the foreseeable future. In many respects, such as the description of binding energies for neutron-rich nuclei, the new interactions already lead to improved results relative to the older USD interaction. We should have more precise theoretical input for astrophysical applications such as those for electron capture [32] and proton capture cross sections [33] where experimental data cannot be obtained. On the other hand, the successes or deficiencies of the theoretical predictions will also give us a better understanding of the precision and limitation of this approach to nuclear structure.

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