ASSIGNMENT OF ERRORS TO CALCULATED TRANSITION MATRIX ELEMENTS

G.A. TIMMER and F. MEURDERS
Fysisch Laboratorium, Rijksuniversiteit, Utrecht, The Netherlands

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Errors are assigned to calculated transition matrix elements to account for uncertainties in the model Hamiltonian. The method is illustrated for the lowest five levels of ^{28}Al for which an excellent correlation is found between the size of the assigned errors and the deviations between theory and experiment.

From two points of view it is desirable to have a measure for the reliability of calculated transition matrix elements. A theorist may be tempted to draw conclusions from a certain theoretical result, which may in fact be meaningless due to uncertainties in the input data on which it is based. An experimentalist would like an "educated guess" for, say, a lifetime before choosing a technique to measure it.

There are three interrelated sources of errors in calculated matrix elements. In the first place the nuclear Hamiltonian is not very well known. In practice there are a number of interactions in use, each of them being able to reproduce a certain amount of experimental data. The main successes of these different interactions do not always involve the same cases. In the second place a truncated Hilbert space must be used. An improper choice of this space may result in the inability to reproduce some experimental results. In the third place the operators used in the chosen truncated space must be renormalized. A common procedure is to assume that the operators can be expressed in a certain analytic form containing a number of parameters that have to be fitted. Examples are the choice of a residual effective interaction in shell model Hamiltonians and an effective charge for the E2 operator.

The main aim of the present paper is to introduce an estimate of the error in calculated transition matrix elements resulting from uncertainties in the Hamiltonian. These uncertainties are reflected in the difference between the calculated and experimental energies.

Let the effective Hamiltonian actually used in the calculation be denoted by H. The eigenvalue equation reads

$$H|K, m\rangle = E_m^K |K, m\rangle, \tag{1}$$

where K denotes the set of quantum numbers of operators like angular momentum that commute with H, independent of the particular choice made for H. The symbol m stands for the eigenvector number within the set labelled by K, such that $E_{m+1}^K \geqslant E_m^K$. The difference between the Hamiltonian used and some other reasonable Hamiltonian will be represented by an extra term δH to be added to H. Hence δH accounts for the uncertainty in H. We assume that H already yields reasonable agreement with experiment, so that the effects of δH may be determined by the aid of perturbation theory. To first order in δH the variation in a matrix element of a transition operator O yields

$$\delta\langle K, m|O|K', m'\rangle = \sum_{i\neq m} \frac{\langle K, m|\delta H|K, i\rangle\langle K, i|O|K', m'\rangle}{E_i^K - E_m^K} + \sum_{i'\neq m'} \frac{\langle K, m|O|K', i'\rangle\langle K', i'|\delta H|K', m'\rangle}{E_{i'}^{K'} - E_{m'}^{K'}}. \tag{2}$$

Problems of possible degeneracy will be ignored.

Since we do not know which δH should give best agreement, we will treat the off-diagonal matrix elements of δH in eq. (2) as uncorrelated random variables. The error assigned to $\langle K, m|O|K', m'\rangle$ is then given by

$$\Delta = \left[\sum_{i\neq m} \left(\frac{\langle K, i|O|K', m'\rangle}{E_i^K - E_m^K} Q_{mi}^K \right)^2 + \sum_{i'\neq m'} \left(\frac{\langle K, m|O|K', i'\rangle}{E_{i'}^{K'} - E_{m'}^{K'}} Q_{m'i'}^{K'} \right)^2 \right]^{1/2}, \tag{3}$$

where Q^K_{mi} is an estimate for the matrix element $\langle K, m|\delta H|K, i\rangle$. Thus Δ^2 is taken to be the incoherent quadratic sum of the terms in eq. (2). Let us take for δH the difference between a Hamiltonian that optimally reproduces the experimental energies and the Hamiltonian used. It then follows from first-order perturbation theory that the diagonal matrix element $\langle K, m|\delta H|K, m\rangle$ is equal to the difference between the experimental and the calculated energy of the state $|K, m\rangle$.

The following ansatz was found to give a reasonable correlation between the size of the resulting error and the agreement between theory and experiment

$$Q^K_{mi} = \frac{1}{2}\left(|E^K_{m\,\mathrm{exp}} - E^K_{m\,\mathrm{calc}}| + |E^K_{i\,\mathrm{exp}} - E^K_{i\,\mathrm{calc}}|\right). \tag{4}$$

Thus the value of the off-diagonal matrix element is replaced by the mean of the absolute values of the corresponding diagonal matrix elements. This ansatz can only be made when we expect the structures of $|K, m\rangle$ and $|K, i\rangle$ not to be very different, since otherwise we are sure to overestimate Q^K_{mi}. An example of a case for which eq. (4) yields a too large matrix element is obtained if the main components of $|K, m\rangle$ and $|K, i\rangle$ have widely different particle distributions, since a one- plus two-body operator like δH will not connect them by a large matrix element. This will occur, however, only for states that show a large difference in energy.

The last step is to neglect the high-lying intermediate states of eq. (3) in the summation. Neither the transition operator nor δH is expected [1] to have large matrix elements to these high-lying states, if we restrict m and m' in eq. (3) to the first few eigenvectors.

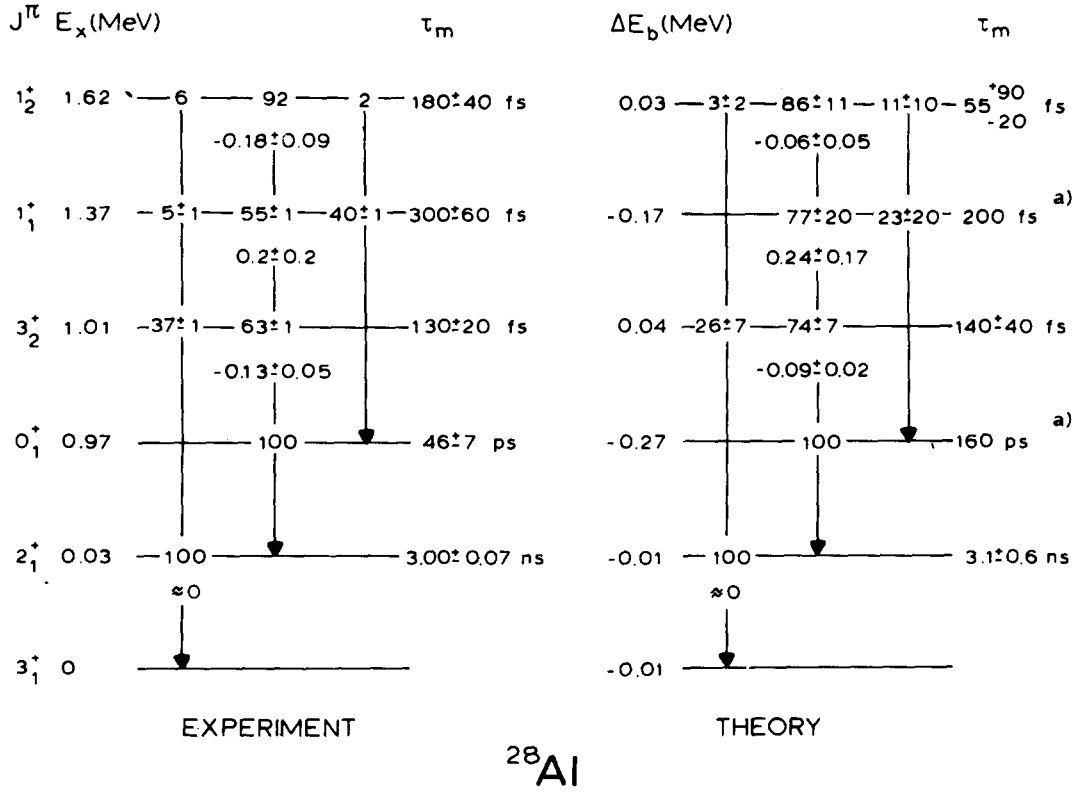

Fig. 1. Lower part of the experimental and calculated decay scheme of ^{28}Al. Lifetimes, branches and E2/M1 mixing ratios are given; ΔE_b represents the difference between the experimental and calculated energies. Experimental data are taken from ref. [3].
a) The calculated error is omitted since it is larger than the value itself.

An interesting fact emerges if one considers the errors in quantities, like mixing ratios, that depend on more than one matrix element. When their variation with δH is written in a form analogous to that of eq. (2), then the dependence on δH is sometimes found to be much weaker than those of the separate matrix elements.

The present technique of error assignment was used extensively in the $A = 24-28$ mass region. The wave functions were obtained [2] in a truncated sd-shell configuration space with a phenomenologically determined effective interaction. For the M1 operator the bare nucleon g-factors were used and for the E2 operator and effective charge of $\Delta e_p = \Delta e_n = 0.55\,e$. As an example we give the results for the decay properties of ^{28}Al in fig. 1. The details of this calculation will be published elsewhere [1]. This figure shows that good agreement is obtained between experiment and theory. Note that the assigned errors give a good estimate of the theoretical accuracy. It can also be seen from the figure that the theoretical lifetimes, branching and mixing ratios have smaller errors and show better agreement with experiment when the energy is well reproduced. The errors assigned to the properties of the 1_2^+ state are large as a consequence of eqs. (3) and (4), since the energy of the 1_1^+ state is badly reproduced. We can thus conclude for this particular example that the configuration space and the transition operators used are sufficiently good to reproduce the data. Small variations in the Hamiltonian should be able to improve the agreement still further. If it should turn out that a calculated transition rate differs markedly from the experimental result, i.e., more than the error resulting from uncertainties in the Hamiltonian allows for, then we may conclude that one of the other possible deficiencies, viz. an improper choice of the configuration space or an improper renormalization of the operators, is responsible.

References

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