AN EFFECTIVE INTERACTION DERIVED FROM SPECTRA AND STATIC MOMENTS

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Received 12 June 1987

A method to derive a phenomenological effective interaction based on energy spectra as well as on static moments of many-particle nuclei is presented. The approach has been applied to $A=4$–16 nuclei. It follows that by including static moments in the input data the agreement with experimental values can be much improved without increasing the number of parameters.

One of the main difficulties in performing large-scale shell-model calculations on the structure of complex nuclei is to find a proper effective nucleon–nucleon interaction. One can use either one of the following methods or a combination of these. (i) The realistic approach, where the hamiltonian is based on nucleon–nucleon scattering data. Although in principle this is the most fundamental solution it is often not accurate enough because of uncertainties in the renormalization procedures required to obtain an effective interaction in a restricted model space. (ii) The phenomenological approach, where the hamiltonian is completely parametrized. A major problem is usually the large number of parameters, e.g. two-body matrix elements, that must be determined from a fit to experimental data. (iii) The schematic approach, where the matrix elements of the hamiltonian are obtained from some effective nucleon–nucleon potential which contains a rather limited set of parameters. This method is often used when the methods (i) and (ii) would cause too many problems.

The p-shell nuclei have been treated with all three methods mentioned above, but none of them appears to reproduce some electromagnetic properties, in particular magnetic dipole moments of $T=1$ nuclei, well enough [1].

In this paper we show that the conventional phenomenological approach, from now on to be denoted by method 1, can be improved considerably. In this respect it is important to realize that of the large variety of experimental data available, only the information on the energies of nuclear states has been used so far to obtain a phenomenological effective interaction. Some well-known examples of this method 1 approach are the early calculations of Cohen and Kurath on p-shell nuclei [2], the recent calculations of Wildenthal et al. [3] on sd-shell nuclei as well as the treatment of p-shell nuclei by Van Hees et al. [4]. In calculations of this type the two-body matrix elements or the Talmi integrals [5], i.e. the weighted integrals over the radial dependence of the nucleon–nucleon potential, are considered as parameters [6]. It is clear from a numerical point of view that, as far as energies are concerned, the highest accuracy can be expected from such a phenomenological interaction. However, the agreement may be partly artificial, since it does not necessarily lead to good wave functions for other observables. This situation can be improved by the present method, in the following to be denoted by method 2. The latter method allows us to use other observables in addition to energy levels as input data for the determination of an optimal hamiltonian. For the additional observables we have selected the static moments, but the formalism can be extended to other observables as well. The method 2 can be summarized as follows.

Starting from first-guess parameter values, we use an iterative procedure to obtain their optimum values. The energy E_k of an eigenstate ψ_k of the hamiltonian H can be expressed in terms of the parameters λ_i as

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(North-Holland Physics Publishing Division)

$$E_k = \langle \psi_k | H | \psi_k \rangle \quad \text{with } H = \sum_i H_i \lambda_i , \tag{1}$$

where the summation ranges over the number of parameters λ_i (e.g. two-body matrix elements). A variation of the parameter values from λ_i to $\lambda_i + \delta\lambda_i$ leads to a first-order change in energy given by

$$\delta E_k = \langle \psi_k | \delta H | \psi_k \rangle \quad \text{with } \delta H = \sum_i H_i \delta\lambda_i , \tag{2}$$

while the first-order change in the wave functions is given by

$$|\delta\psi_k\rangle = \sum_{l \neq k} |\psi_l\rangle \frac{\langle \psi_l | \delta H | \psi_k \rangle}{E_l - E_k} . \tag{3}$$

The summation over l includes in principle all eigenstates of H.

Similarly one can express a static moment m_l of a state ψ_l in terms of the parameters μ_j of the electromagnetic moment operator M as

$$m_l = \langle \psi_l | M | \psi_l \rangle \quad \text{with } M = \sum_j M_j \mu_j , \tag{4}$$

where the summation ranges over the number of parameters μ_j (e.g. effective nucleon g-factors and/or effective charges). A change of μ_j to $\mu_j + \delta\mu_j$ results in a change Δm_l in the calculated moment which is given by

$$\Delta m_l = \langle \psi_l | \delta M | \psi_l \rangle \quad \text{with } \delta M = \sum_j M_j \delta\mu_j . \tag{5}$$

A simultaneous variation in the hamiltonian parameters λ_i and in the parameters μ_j of the moment operators modifies the static moments in first order to

$$m_l + \delta m_l = \langle \psi_l | M | \psi_l \rangle + \langle \psi_l | \delta M | \psi_l \rangle + 2 \langle \delta\psi_l | M | \psi_l \rangle . \tag{6}$$

Substituting expressions (2)–(5) into eq. (6) one finds

$$m_l + \delta m_l = \sum_j \langle \psi_l | M_j | \psi_l \rangle \, (\mu_j + \delta\mu_j) + 2 \sum_i \sum_{k \neq l} \frac{\langle \psi_k | H_i | \psi_l \rangle}{E_k - E_l} \langle \psi_k | M | \psi_l \rangle \, \delta\lambda_i . \tag{7}$$

In a least-squares fit, which includes experimental energies as well as static moments, one minimizes Q^2 given by

$$Q^2 = \sum_k w_k^2 (E_k + \delta E_k - E_k^{\text{exp}})^2 + \sum_l w_l^2 (m_l + \delta m_l - m_l^{\text{exp}})^2 , \tag{8}$$

where w_l and w_k are the weight factors for the energies and moments, respectively. The values for $\lambda_i + \delta\lambda_i$ and $\mu_j + \delta\mu_j$ obtained from this fit are used again as starting values for the next iteration step. This procedure is repeated till convergence is reached, which usually takes less than five iteration steps. In the present rather restricted $(0+1)\hbar\omega$ model space for p-shell nuclei we assigned the weight factors such that the average contributions of energies and moments to Q^2, see eq. (8), are of comparable magnitude.

The conventional method 1 can be formulated rather easily within the present outline of method 2. Therefore one only has to replace δm_l in eq. (8) by Δm_l which is defined in eq. (5). In this case the minimization of Q^2 can be performed in two steps since the static moments do no longer influence the parameters λ_i of the hamiltonian. The first step determines the parameters λ_i from the energy levels and hence fixes the wave functions. The second step determines the effective g-factors and charges from the static moments while keeping the wave functions fixed.

The method 2 has been applied to the $A=4$–16 p-shell nuclei in a no-core $(0+1)\hbar\omega$ model space. The experimental data used as input in the fitting procedure contain about 150 binding energies of ground states and excited states and the ~ 40 known static moments of which the majority consists of magnetic dipole moments. With this set of nearly 200 experimental data we determined (i) the parameters for the effective interaction expressed in terms of 21 phenomenological Talmi integrals which can contribute in the $(0+1)\hbar\omega$ model space [6], (ii) the value of $\hbar\omega$ and (iii) the effective nucleon g-factors and electric charges.

It follows from the sum over k in eq. (7) that all eigenvectors ψ_k of a given hamiltonian should be included. This would require the complete diagonalization of the corresponding matrices, which for a large model space becomes extremely involved. Hence, it is of practical importance to investigate whether convergence of the iteration procedure can

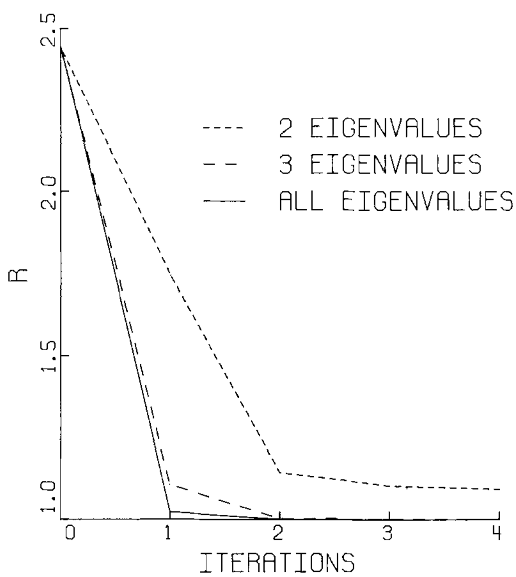

Fig. 1. The ratio $R = Q^2/Q^2_{\mathrm{min}}$ defined in eq. (8), as a function of the number of iteration steps when two (a), three (b) or all (c) eigenvectors are taken into account for each matrix used in the least-squares fit.

be obtained by including only the lower-lying states of each matrix. The main results of this investigation are presented in fig. 1. The value of Q^2, see eq. (8), relative to its value Q^2_{min} reached after comvergence, is given as a function of the number of iteration steps when two, three or all eigenstates of the matrices involved are taken into account. Fig. 1 shows that convergence is reached very fast, even when only the lower three eigenvectors of a matrix are included. We found that the results obtained for Q^2_{min} are not influenced by this restriction of the summation over k, except when we restrict the summation to $k=2$ only. It should be noted that the "first-guess" parameters used here are converged ones obtained from the fit with method 1. Another result of practical interest is that the inclusion of static moments in the least-squares fit increases computer time for one iteration by no more than a factor of 1.5. Preliminary results obtained in much larger model spaces confirm these findings.

It is interesting to make a comparison between the results obtained from the traditional energy fit (method 1) and the present approach which also includes static moments (method 2). Each method is applied to the same set of experimental data, while in both cases the same number of parameters is used. A summary of the main results of this comparison is given below.

(i) The hamiltonian parameters (21 Talmi integrals and the value of $\hbar\omega$) are better determined by method 2 in particular the $T=0$ tensor part of the interaction.

(ii) Method 2 yields effective g-factors which deviate considerably less from the bare-nucleon values than those of method 1. This is illustrated in table 1, where the effective g-factors and electric charges are compared with the bare-nucleon values. The effective g-factors and charges for method 1 are obtained in the traditional way, i.e. from a separate fit of nucleon g-factors to the static moments, while keeping the hamiltonian and thus the wave functions fixed to those obtained from the fit to energy levels only.

(iii) The deviations between calculated and measured magnetic dipole moments become very small

Table 1
Parameters of the M1 and E2 operators.

Nucleon g-factors and electric charges		Method 1 [a]	Method 2 [b]	Bare-nucleon value
protons	g^l	1.25	1.03	1.00
	g^s	5.36	5.54	5.59
		1.33	1.26	1.00
neutrons	g^l	−0.16	0.04	0.00
	g^s	−3.62	−3.88	−3.83
	e	0.32	0.47	0.00

[a] Only level energies are used for phenomenological interaction.
[b] Levels and static moments are used for phenomenological interaction.

Table 2
The $T=1$ magnetic dipole moments (n.m.) in p-shell nuclei.

Nucleus	J^π	Theory		Experiment
		method 1	method 2	
^{8}Li	2^+	1.52	1.61	1.65
^{8}B	2^+	1.21	1.02	1.04
^{12}B	1^+	0.63	0.90	1.00
^{12}N	1^+	0.78	0.47	0.46
^{14}C	3^-	−0.65	−0.79	±0.82
^{16}N	3^-	−1.63	−1.54	±1.60
^{16}N	1^-	−1.27	−1.73	−1.83

Table 3
Calculated magnetic dipole moments of nonnormal-parity states with $\tau_m > 1$ ps.

Nucleus	J^π; T	E_x (MeV)	μ (method 2)
^{11}Be	$1/2^+$; 3/2	0	−1.47
^{14}B	2^-; 2	0	+1.46
^{14}N	3^-; 0	5.83	+1.78
^{15}C	$1/2^+$; 3/2	0	−1.66
^{16}N	2^-; 1	0	−2.78

with method 2. The average absolute deviation between calculated and experimental magnetic dipole moments reduces from 0.18 (method 1) to 0.06 (method 2). For the $T=1$ states with an experimentally known magnetic dipole moment results are given in table 2. Values calculated according to method 2 for the nonnormal-parity states with a known rather long lifetime of more than 1 ps, but which have not been measured so far, are presented in table 3.

(iv) The quadrupole moments are only slightly improved by method 2, with Δe (neutron) considerably larger tha Δe (proton), see table 1.

(v) As stated before the agreement for energies can only become worse with method 2 because additional data on other observables have been included in the fit without increasing the number of parameters. It turns out, however, that the average RMS deviation between calculated and experimental energies increases by no more than about 10%.

Summarizing we have shown that a phenomenological effective nucleon–nucleon interaction based on experimental data, which include energies as well as static moments of many-particle nuclei can be derived quite efficiently. The new approach (method 2) strongly improves the agreement with magnetic dipole moments without increasing the number of parameters. This procedure may therefore become useful for a more critical study of possible effects of a nonnucleonic nature. A more detailed account of the results obtained with the present approach will be published elsewhere.

This work was performed as part of the research program of the "Stichting voor Fundamenteel Onderzoek der Materie" (FOM) with financial support from the "Nederlandse Organisatie voor Zuiver-Wetenschappelijk Onderzoek" (ZWO).

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