Information on effective interactions from experimental single-particle energies

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A method is presented for obtaining centroids of the effective nucleon-nucleon interaction directly from measured single-particle energies. An application to nuclei in the mass region $A=28$ to 56 is provided to illustrate the technique. Uncertainties in the centroids are estimated at 100 keV or less, except in cases of exceptional fragmentation of the single-particle strength. Methods such as the one proposed here can be used to place constraints on realistic interactions calculated from bare nucleon-nucleon potentials, which are known to possess defective centroids in many cases.

To carry out any nuclear structure calculation, a Hamiltonian must first be constructed; with the usual assumptions, this is formed from two-body matrix elements of an effective interaction, which therefore form an essential input to such calculations. Unfortunately, there are many problems associated with the construction of a Hamiltonian which is sufficiently accurate for spectroscopic calculations. As an example, the deficiencies of realistic interactions such as those produced by Kuo and Brown[1,2] are well known: In *sd*-shell nuclei these interactions lead to the phenomenon of band shifting,[3-5] whereas in the *fp* shell groups of energy levels are shifted relative to states of different dominant configuration.[6-8] Both of the problems can be traced to incorrect centroids of the interaction between particles in different orbitals, and this defect is in fact particularly acute when the orbitals are in different major shells. This is especially unfortunate in view of the recent revival of interest in the properties of extremely neutron-rich or proton-rich nuclei (see, for example, Refs. 9–11) and in the effects of core breaking.[12,13]

Because of the problems associated with the construction of realistic interactions, most nuclear structure studies employ effective interactions which are to some extent fitted to experimental data, thereby minimizing inaccuracies in centroids. The aim of the present work is somewhat more limited than a full fit—namely, to extract directly from experimental data information on the centroids themselves. It is obvious that values for individual two-body matrix elements of the interaction can be deduced from the spectra of nuclei with two nucleons relative to an inert core—for a recent review see Ref. 14; it is perhaps less obvious that useful information about effective interactions is available from single-particle spectra, by comparing single-particle energies relative to different inert cores. For example, the energies of a single nucleon in the $f_{7/2}$ orbit measured relative to ^{32}S and ^{40}Ca differ since the latter energy contains an additional contribution from the interaction of the $f_{7/2}$ nucleon and the fully occupied $d_{3/2}$ orbit. Comparison of the energies of the relevant $\frac{7}{2}^-$ states of ^{33}S and ^{41}Ca therefore yields information concerning the $f_{7/2}$-$d_{3/2}$ interaction.

Consider a nucleus with n_p and n_q active nucleons in orbitals p and q, respectively. The average energy of this configuration, relative to the inert core A_0, is[8]

$$E(n_p,n_q)=n_p\epsilon_p+n_p(n_p-1)\bar{V}(pp)/2+n_q\epsilon_q+n_q(n_q-1)\bar{V}(qq)/2+n_pn_q\bar{V}(pq)\ . \tag{1}$$

In Eq. (1), the ϵ_i are single-particle energies relative to the inert core A_0 and the interaction centroids $\bar{V}(ij)$ are given by

$$\bar{V}(ij)=\frac{\sum_{JT}(2J+1)(2T+1)V^{JT}(ij)}{\sum_{JT}(2J+1)(2T+1)}\ , \tag{2}$$

where the $V^{JT}(ij)=\langle ij|V|ij;JT\rangle$ are diagonal matrix elements of the effective interaction for spin J and isospin T. It follows from Eq. (1) that, relative to the inert core A_0' with orbit p completely filled with $N_p=2j_p+1$ neutrons and an equal number of protons, the energy of a single nucleon in any orbital q is

$$\epsilon_q(A_0')=\epsilon_q(A_0)+(2N_p-\delta_{pq})\bar{V}(pq)\ . \tag{3}$$

If q refers to an orbital below the Fermi energy of the core $A_0'=A_0+2N_p$, then $\epsilon_p(A_0')$ is to be interpreted as a single-hole energy.

If, however, the core A_0' is produced by closure of different neutron and proton shells, i.e., N_p identical nucleons occupy the orbit p so that $A_0'=A_0+N_p$, then proper account must be taken of isospin. In particular, Eq. (1) is replaced by[8]

$$E(n_p,n_q;T_p,T_q;T)=E_p(n_p,T_p)+E_q(n_q,T_q)+n_pn_qa_{pq}+[T(T+1)-T_p(T_p+1)-T_q(T_q+1)]b_{pq}/2 \tag{4}$$

where, for example,

$$E_p(n_p,T_p)=n_p\epsilon_p+n_p(n_p-1)a_{pp}/2+[T_p(T_p+1)-3n_p/4]b_{pp}/2\ . \tag{5}$$

The parameters of Eqs. (4) and (5) are related to various interaction centroids by, for example,

$$\bar{V}^{T=1}(pq)=a_{pq}+b_{pq}/4\ ,$$
$$\bar{V}^{np}(pq)=a_{pq}-b_{pq}/4\ , \tag{6}$$

for $p\neq q$. These additional centroids are defined by equations similar to Eq. (2):

$$\bar{V}^{T}(pq)=\frac{\sum_J (2J+1)V^{JT}(pq)}{\sum_J (2J+1)}\ , \tag{7}$$

and

$$\bar{V}^{np}(pq)=\frac{\sum_J (2J+1)V^{J}(pq)}{\sum_J (2J+1)}\ ; \tag{8}$$

the sums over J include matrix elements for fixed T and all T for the isospin and neutron-proton centroids, respectively.

Assuming for definiteness that the nucleons in orbit p are neutrons, then single-particle states can be constructed from the core $A_0'=A_0+N_p$ by adding a neutron to any orbit q above the Fermi level or by removing a neutron from the orbital p. The energy of such a state, relative to the inert core A_0', is

$$\epsilon_q^{\nu}(A_0')=\epsilon_q(A_0)+(N_p-\delta_{pq})\bar{V}^{T=1}(pq)\ , \tag{9}$$

where the suffix ν indicates a *neutron* coupled to a *neutron-rich* core. Further single-particle states are formed by removing a *proton* from below the Fermi level of the core A_0' or placing a *proton* in the orbital p; the energy of these states, relative to the core A_0', is given by

$$\epsilon_q^{\pi}(A_0')=\epsilon_q(A_0)+N_p\bar{V}^{np}(pq)\ . \tag{10}$$

Other single-particle states can be constructed, by adding protons or removing neutrons above and below the Fermi level, respectively, but it is, for various reasons, difficult to extract reliable estimates for centroids using these states. For example, adding a *proton* to an orbit above the *neutron* Fermi level does not usually produce a state of good isospin: States of isospin $T_{\rm core}\pm\frac{1}{2}$ can usually be constructed. The proton single-particle state of higher isospin is the isobaric analog of the corresponding neutron state and its analysis yields no additional information, assuming charge independence of the effective nuclear interaction. The state of lower isospin, the antianalog state, is (like the analog state) in fact a linear combination of the proton single-particle state and a neutron state. Analysis of the antianalog and analog states, suitably combined with the appropriate isospin coupling coefficients, yields an estimate of the centroid $\bar{V}^{np}(pq)$. Unfortunately, as it known from studies[15,16] with the weak-coupling model of Bansal and French,[17] the states of lower isospin are poorly described by such models, leading to additional uncertainties in the values of centroids extracted; such states will therefore not be considered here.

Special cases of Eqs. (3), (9), and (10) have been presented previously[2,18,19] (and their structure is perhaps intuitively obvious), although they are usually employed to compute single-particle energies relative to a new core for a given effective interaction. The intention here is that the equations should be used instead to compute interaction centroids from measured single-particle energies. The energies ϵ_q are extracted from experimental binding energies $B(A,J^{\pi})$:

$$\epsilon_q(A_0)=\pm[B(A_0\pm1,J^{\pi}=j_q^{\pi})-B(A_0,0^{+})]\ , \tag{11}$$

for a single particle and a single hole, respectively. The validity of this technique, and the accuracy of the centroids extracted, rests on the assumption of shell closure—a convenient indicator of this (in addition to the excitation energy of the first excited state in the closed-shell nuclei) is the degree of fragmentation of the associated single-particle states. In determining single-particle energies through Eq. (11), we have taken the binding energy of the state of the $A_0\pm1$ nucleus with largest spectroscopic strength (usually greater than 60%), rather than the average energy weighted with measured spectroscopic factors. The average single-particle strength typically lies about 0.3 MeV above the energy used, but since we are interested in differences in single-particle energies this systematic error should cancel approximately. Moreover, since the energy difference is ultimately divided by a factor such as $2N_p$, the uncertainty in the centroids due to fragmentation is probably less than 100 keV, apart from in a few exceptional cases.

To illustrate the proposed technique, we present a simple application. We consider single-particle states in the mass range $A=28$–56, with the orbitals $2s_{1/2}$, $1d_{3/2}$, and $1f_{7/2}$ active. The ground states of ^{28}Si, ^{32}S, ^{40}Ca, and ^{56}Ni are assumed to comprise closed shells; in addition, the ground states of ^{30}Si/S, ^{36}S/Ca, and ^{48}Ca are regarded as inert cores with $N\neq Z$. The single-particle and hole energies computed using Eq. (11) and data from Refs. 20 and 21 are listed in Table I. Where necessary, the Coulomb contribution to experimental binding energies has been extracted using the approximate procedures of Refs. 22 and 23; this could introduce additional uncertainties of up to 0.3 MeV in some values of ϵ_q^{π}. Core breaking, in any case, leads occasionally to even larger uncertainties. For example, the $f_{7/2}$ single-particle state in ^{29}Si and the $s_{1/2}$ hole strength in ^{47}K are both evidently highly fragmented; the uncertainty in the value of ϵ_q probably exceeds 0.5 MeV. In many cases, experimental spectroscopic factors are unavailable, making it difficult to estimate uncertainties in the extracted centroids.

Interaction centroids extracted using Eqs. (3), (9), and (10) and the single-particle energies of Table I are listed in Table II. Values of the centroids of the $s_{1/2}$-$f_{7/2}$ interaction are adversely affected by the exceptional fragmentation mentioned above; correcting for this would probably reduce the centroids $\bar{V}(sf)$ and $\bar{V}^{np}(sf)$ by about 0.2 MeV and $\bar{V}^{T=1}(sf)$ by as much as 0.4 MeV. In three cases, the centroid $\bar{V}(pq)$ can be obtained independently from two sets of data. The two estimates of $\bar{V}(sd)$ and $\bar{V}(df)$ differ by only 25 keV, whereas values of $\bar{V}(sf)$ obtained from cores $(A_0,A_0')=(28,32)$ and (40,56) differ by 100 keV. A further indication of the uncertainties inherent in the method is provided by the results for

TABLE I. Experimental single-particle and single-hole energies. Single-hole energies are designated by an asterisk.

$\epsilon_q(A_0)$			
A_0	$s_{1/2}$	$d_{3/2}$	$f_{7/2}$
28	−8.47	−7.20	−4.85
32	−15.04*	−8.64	−5.71
40	−18.11*	−15.64*	−8.36
56	−19.83*	−20.39*	−16.64*
$\epsilon_q^{\nu}(A_0)$			
A_0	$s_{1/2}$	$d_{3/2}$	$f_{7/2}$
30	−10.61*	−6.59	−3.45
36		−9.89*	−4.30
48			−9.95*
$\epsilon_q^{\pi}(A_0)$			
A_0	$s_{1/2}$	$d_{3/2}$	$f_{7/2}$
30	−13.05		
36	−18.96*	−14.79	
48	−23.63*	−23.53*	−16.86

TABLE II. Interaction centroids.

$\bar{V}(pq)$			
pq	Kuo-Brown[a]	WBMB[b]	Present work
ss	−2.57	−2.12	−2.19
dd	−0.74	−0.90	−1.00
ff	−0.44	−0.69	−0.55
sd	−0.65	−0.56	−0.37
df	−0.42	−0.58	−0.32
sf	−0.20	−0.50	−0.16
$\bar{V}^{np}(pq)$			
pq	Kuo-Brown[a]	WBMB[b]	Present work[c]
ss	−2.87	−2.34	−2.29(−2.22)
dd	−1.24	−1.33	−1.54(−1.44)
ff	−0.70	−1.06	−1.06(−0.84)
sd	−1.18	−1.09	−0.98(−1.05)
df	−0.80	−1.17	−0.99(−0.98)
sf	−0.53	−0.86	−0.70(−1.02)
$\bar{V}^{T=1}(pq)$			
pq	Kuo-Brown[a]	WBMB[b]	Present work
ss	−1.95	−1.67	−2.14
dd	−0.07	−0.33	−0.42
ff	−0.13	−0.27	−0.23
sd	−0.12	−0.02	0.31
df	−0.05	0.02	0.35
sf	0.14	−0.14	0.69

[a]Centroids of Kuo-Brown interactions (Refs. 1 and 2).
[b]Centroids of WBMB interaction (Ref. 10).
[c]Centroids in parentheses are computed from other centroids; the others are extracted directly from data.

$\bar{V}^{np}(pq)$. The values in parentheses in Table II, obtained by suitably combining $\bar{V}(pq)$ and $\bar{V}^{T=1}(pq)$, differ on average by 100 keV from the values deduced directly using Eq. (11).

Also listed in Table II are centroids of the hybrid interaction of Warburton, Becker, Millener, and Brown (WBMB).[10] Parts of this interaction are fitted to nuclear level schemes, but in different model spaces; they are therefore differently renormalized. The (df) interaction has been adjusted to fit certain states of ^{40}Ca, while the (sf) interaction is unfitted. Comparison with the results of the present work reveals surprising agreement in most cases, although values of $\bar{V}(p\neq q)$ and $\bar{V}^{T=1}(p\neq q)$ differ significantly, in that the WBMB interaction is approximately 0.3 MeV more attractive. For further comparison, centroids of the realistic interactions of Kuo and Brown[1,2] are also presented in Table II. Again, different centroids are appropriate to different model spaces, making direct comparison more difficult. There are, however, several instances in which the Kuo-Brown centroids are substantially different from both the other estimates.

In summary, we have presented a simple technique for extracting information about effective interactions directly from experimental data. Since the data are in fact single-particle spectra, the centroids so obtained should be regarded as supplementing the more extensive information provided by methods involving two-particle spectra.[14] The uncertainty in the values extracted attributable to fragmentation of the single-particle strength is perhaps less than 100 keV in most cases; the extra effort required to reduce this source of error is probably not justified. The centroids produced by the present technique can be used to place constraints on realistic interactions, such as those of Kuo and Brown.

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