Center-of-mass effects in single-nucleon knock-out reactions

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Center-of-mass corrections for quantities observed in single-nucleon knock-out reactions like $(e, e'p)$ are discussed. Explicit results are obtained for the momentum distributions, occupation probabilities, and single-particle energies in the framework of the harmonic oscillator model.

1. INTRODUCTION

The primary motivation for performing coincidence experiments such as $(e, e'p)$ and $(p, 2p)$ is that such knock-out reactions provide[1,2] a rather direct means of investigating the single-particle structure of the nucleus. In the independent-particle model one directly measures the single-particle energies and momentum distributions (and thus essentially the wave function). For more realistic models similar information about the properties of the initial nucleus can be obtained by performing a partial sum over final states to form the hole state. By taking the contribution of all final states into account one can also construct a sum rule[3] for the total binding energy. This is of particular interest, since while this sum rule is very general it does depend on the assumption that there are no three-body forces.

Strictly speaking, such a simple and direct interpretation of knock-out reactions is only possible in plane wave impulse approximation (PWIA), and for a quantitative analysis the appropriate corrections to this approximation must be applied. The calculation of such corrections in a theoretically reliable way is an important but very difficult problem and will not be considered in this paper.

The results of knock-out reactions are usually interpreted[1,2] in the independent-particle model which does not satisfy translational invariance. Moreover, this difficulty generally persists in more sophisticated theories. In this paper we discuss what effects, i.e., center of mass (c.m.) corrections, the imposition of this symmetry (on the nuclear wave function) gives.

In Sec. 2 we review the formalism for knock-out processes. In Sec. 3 we consider the special case of c.m. corrections to the binding energy sum rule which does not require a model. Though basically a $1/A$ effect, the net correction is increased by the large cancellation of the kinetic and potential energy contributions. The c.m. corrections for the momentum distributions, occupation probabilities, and single-particle energies are discussed in the last section in the framework of the harmonic oscillator model (for the wave functions). Here, the c.m. corrections basically arise from the spurious components of the shell model hole state. For example, the 20% "spuriosity" of the $0s$ hole state in ^{16}O represents components that are actually in a $0p$ hole state in the intrinsic wave function. One thus finds a 20% reduction of the $0s$ strength and a corresponding increase in the $0p$ strength. These components also lead to a spurious contribution to single-particle energy of the $0s$ state from the $0p$ state. Correcting for this effect, one finds an increased binding for the $0s$ state. Technical details such as the construction of the nonspurious hole state wave functions are handled in the Appendixes.

2. CROSS SECTION FOR KNOCK-OUT REACTIONS

In plane wave impulse approximation the cross section for quasielastic knock-out processes[1,2,4,5] such as $(e, e'p)$ and $(p, 2p)$ is proportional to the spectral function

$$P(\vec{k}, E) = \sum_i |A_i(\vec{k})|^2 \delta(E - E^i_{A-1} + E_A), \tag{2.1}$$

where E and $\vec{k}$ are the energy and momentum transferred to the nucleus by the projectile a, and outgoing particles b and c:

$$\begin{aligned} E &= E_a - E_b - E_c, \\ \vec{k} &= \vec{k}_a - \vec{k}_b - \vec{k}_c. \end{aligned} \tag{2.2}$$

E_A is the binding energy of the target nucleus and E^i_{A-1} the energy of the $A-1$ nucleus in final state i (in the laboratory frame). The amplitude $A_i(\vec{k})$ is the Fourier transform of the overlap integral of the initial and final nuclear wave functions (in the laboratory frame)

$$A_i(\vec{k}) = \int d\vec{r}_A \, e^{i\vec{k}\cdot\vec{r}_A} \langle \psi^i_{A-1} | \psi_A \rangle, \tag{2.3}$$

where

$$\langle \psi^i_{A-1} | \psi_A \rangle = \sqrt{A} \int d\vec{r}_1 \cdots d\vec{r}_{A-1} \psi^{i*}_{A-1}(\vec{r}_1 \cdots \vec{r}_{A-1}) \psi_A(\vec{r}_1 \cdots \vec{r}_A) . \tag{2.4}$$

Physically $|A_i(\vec{k})|^2$ represents the momentum distribution of the nucleon in the initial state before it was knocked out. To simplify the formalism explicit spin and isospin labels have been suppressed.

In these expressions all quantities are defined in the laboratory frame and no explicit use of translational invariance has been made. Imposing the latter it is more convenient to reexpress them in terms of the corresponding intrinsic quantities. Noting that the residual nucleus recoils with momentum $\vec{k}$ we have

$$E^i_{A-1} = E^i_{A-1,\,\mathrm{int}} + \frac{k^2}{2(A-1)m} , \tag{2.5}$$

and

$$\langle \psi^i_{A-1} | \psi_A \rangle = \frac{1}{\Omega} \int d\vec{R}' e^{-i\vec{k}\cdot\vec{R}'} \langle \psi^i_{A-1} | \psi_A \rangle_{\mathrm{int}} , \tag{2.6}$$

where $\vec{R}' = [1/(A-1)] \sum_{i=1}^{A-1} \vec{r}_i$ is the c.m. coordinate of the residual $A-1$ nucleus and Ω is the normalization volume. We thus find

$$P(\vec{k}, E) = \sum_i |A_i(\vec{k})|^2 \delta\left(E + \epsilon_i - \eta \frac{k^2}{2m}\right) , \tag{2.7}$$

and

$$A_i(\vec{k}) = \int d\vec{r}'_A e^{i\vec{k}\cdot\vec{r}'_A} \langle \psi^i_{A-1} | \psi_A \rangle_{\mathrm{int}} , \tag{2.8}$$

with

$$\eta = \frac{1}{A-1} , \qquad \vec{r}'_i = \vec{r}_i - \vec{R}' , \qquad \epsilon_i = E_A - E^i_{A-1,\,\mathrm{int}} . \tag{2.9}$$

Although this formulation is exact, since it requires translational invariance, it is not directly applicable to most nuclear structure calculations. In particular we note that $\langle \psi^{(i)}_{A-1} | \psi_A \rangle_{\mathrm{int}}$ is in general not even defined, and thus (2.3) is often used instead of (2.8). The goal of this paper is to determine how the imposition of this symmetry on the nuclear structure affects the theoretical predictions for knock-out reactions.

In the extreme independent-particle model such knock-out processes allow one to measure directly the energies and momentum distributions of the single-particle wave functions in the initial state. In more realistic situations, however, the hole strength is distributed among various eigenstates of the final nucleus. We therefore introduce the concept of single-particle occupation probabilities and energies which will be used in the following sections.

Expanding the intrinsic ground state wave function ψ_A in a complete set of orthonormal single-particle orbitals $\phi_\alpha(\vec{r}'_{A-1})$

$$\psi_A = \frac{1}{\sqrt{A}} \sum_\alpha \psi^\alpha_{A-1}(\vec{r}'_1 \cdots \vec{r}'_A) \phi_\alpha(\vec{r}'_A) , \tag{2.10}$$

the spectral function (2.7) takes the form

$$P(\vec{k}, E) = \sum_{\alpha\beta} \phi^*_\alpha(\vec{k}) \phi_\beta(\vec{k}) \times \sum_i S^i_{\alpha\beta} \delta\left(E + \epsilon_i - \eta \frac{k^2}{2m}\right) , \tag{2.11}$$

where

$$S^i_{\alpha\beta} = \langle \psi^\alpha_{A-1} | \psi^i_{A-1} \rangle \langle \psi^i_{A-1} | \psi^\beta_{A-1} \rangle . \tag{2.12}$$

One can then define occupation probabilities

$$S_{\alpha\beta} = \sum_i S^i_{\alpha\beta} = \langle \psi^\alpha_{A-1} | \psi^\beta_{A-1} \rangle , \tag{2.13}$$

and single-particle removal energies[3,6]

$$\epsilon_\alpha = \frac{1}{S_{\alpha\alpha}} \sum S^i_{\alpha\alpha} \epsilon_i = \langle \psi_A | H | \psi_A \rangle - \frac{1}{S_{\alpha\alpha}} \langle \psi^\alpha_{A-1} | H | \psi^\alpha_{A-1} \rangle , \tag{2.14}$$

which depend only on the ground state wave function of the initial nucleus and the Hamiltonian H.

3. SUM RULES

By integrating over the spectral function and using closure one obtains the spectroscopic sum rule

$$A = \int d\vec{k} \int dE\, P(\vec{k}, E) = \sum_\alpha S_{\alpha\alpha} , \tag{3.1}$$

which simply follows from the normalization requirement. Since this sum rule is rather trivial its main usefulness lies not in the basic physics of the knock-out processes itself, but is that it provides a check on whether the corrections to PWIA have been carried out properly, and whether the total strength has been exhausted experimentally. More interesting is the energy-weighted sum rule[3,6]

$$E_A = \frac{1}{2} \int d\vec{k} \int dE \left(-E + \frac{k^2}{2m}\right) P(\vec{k}, E) , \tag{3.2}$$

which is very general only relying on the assumption that the Hamiltonian $H = T + V$ contains only two-body forces. An accurate experimental check

of this sum rule would be of extreme interest, for a violation could give direct evidence for the existence of three- or more-body forces.

We note that the energy E in (3.2) is the energy transfer as measured in the laboratory frame, and not the intrinsic energy transfer, $E_{\rm int} = E - \eta(k^2/2m)$, in terms of which such experiments are usually analyzed. In terms of $E_{\rm int}$ the sum rule reads

$$E_A = \frac{1}{2}\int d\vec{k}\int dE_{\rm int}\left[-E_{\rm int} + (1-\eta)\frac{k^2}{2m}\right] P(\vec{k}, E)\,. \tag{3.3}$$

Equivalently the sum rule can be expressed in a single-particle basis as

$$E_A = \frac{1}{2}\sum_{\alpha} S_{\alpha\alpha}\epsilon_{\alpha\alpha} + \tfrac{1}{2}(1-\eta)T\,, \tag{3.4}$$

where

$$T = \sum_{\alpha\beta} S_{\alpha\beta}\left\langle \phi_\beta \left| \frac{p^2}{2m} \right| \phi_\alpha \right\rangle. \tag{3.5}$$

In this form the c.m. correction factor $1-\eta = (A-2)/(A-1)$ associated with $\frac{1}{2}T$ can be seen to be necessary to cancel the extra kinetic energy in ϵ_α arising from the reduced mass effect $m/m^* = 1+\eta$. The reader can easily justify the need for such a correction by considering the case of the deuteron for which $E_A = \epsilon_i$.

As an application of the sum rule (3.3) we mention a recent $(e, e'p)$ experiment on ^{12}C by the Saclay group.[7] The binding energy per proton obtained from the right-hand side of (3.2) was found to be 4.0 MeV (of which 0.8 MeV comes from the term $-\frac{1}{2}\eta T$), compared with 6.9 MeV obtained from nuclear masses and appropriate Coulomb corrections.

4. CENTER-OF-MASS CORRECTIONS FOR HOLE STATES

Since most theoretical nuclear structure calculations are carried out in the framework of the shell model, the results are affected by the unphysical c.m. motion. Of the various physical quantities involved in knock-out processes only for the binding energy have c.m. corrections been studied[8-10] in any detail. In this section we study the c.m. corrections for the momentum distributions, occupation probabilities and single-particle energies and show that these corrections are in fact necessary in order to satisfy the (c.m. corrected) energy-weighted sum rule (3.4).

In order to define the concept of a c.m. correction it is necessary to have a shell model theory to which there corresponds a unique or physically understood intrinsic analog. The simplest such model which we shall use here is that of harmonic oscillator (HO) wave functions.[11] In the shell model this roughly corresponds with Hartree-Fock (HF) theory. For light nuclei where the c.m. corrections are the largest, the restriction to HO wave functions is a fairly good approximation. We also note that the definition of the single-particle energies ϵ_α (2.14) is consistent with HF theory.

Although we do not assume HO forces, in order to determine the appropriate form of the intrinsic wave function, it is useful to use the fact that the intrinsic HO wave function is the exact solution of the A-body problem with HO internucleon forces:

$$V_{\rm HO}^{\rm int} = V_{\rm HO}^{\rm SM} - V_{\rm HO}^{\rm c.m.} = \sum_i \frac{\omega}{2b^2} r_i^{\,2} - \frac{\omega}{2b^2} AR^2$$

$$= \sum_i \frac{\omega}{2b^2}(\vec{r}_i - \vec{R})^2 = \sum_{i<j} \frac{\omega}{2b^2}\frac{1}{A}(\vec{r}_i - \vec{r}_j)^2\,, \tag{4.1}$$

where $b = (m\omega)^{-1/2}$ and $\vec{R} = (1/A)\sum_{i=1}^{A}\vec{r}_i$.

Furthermore it is the very special nature of HO forces that groups of particles only interact dynamically through their c.m.'s. This can be seen by rewriting

$$V_{\rm HO}^{\rm int} = \frac{\omega}{2b^2}\frac{A-1}{A}(\vec{r}_A - \vec{R}')^2 + \sum_{i=1}^{A-1}\frac{\omega}{2b^2}(\vec{r}_i - \vec{R}')^2\,, \tag{4.2}$$

which immediately implies that the (unantisymmetrized) wave function can be expressed as

$$\psi_A(\vec{r}_1' \cdots \vec{r}_A') = \psi_{A-1}^{\alpha}(\vec{r}_1' \cdots \vec{r}_{A-1}')\phi_\alpha(\vec{r}_A')\,. \tag{4.3}$$

Taking into account the reduced mass corresponding to the relative coordinate $\vec{r}_A - \vec{R}'$, $m^* = [(A-1)/A]m$, one finds that ϕ_α is an HO wave function, but with a modified oscillator parameter: $b' = [A/(A-1)]^{1/2}b$. The c.m. correction for the momentum distribution is thus simply given by $b \to [A/(A-1)]^{1/2}b$.

We now proceed to develop the expansion (2.10). In the shell model the HO single-particle wave function has the form

$$\phi^{\rm HOSM}(\vec{r}) = b^{-3/2}p_\alpha(\vec{r}/b)\exp\left(-\frac{r^2}{2b^2}\right). \tag{4.4}$$

The index α denotes the set of quantum numbers necessary to specify the single-particle state; p_α is a polynomial in $\vec{r}$ of order m_α, the oscillator shell number $[e_\alpha^{\rm HO} = (m_\alpha + \frac{3}{2})\omega]$, and implicitly includes the spin and isospin dependence. The

intrinsic ground state wave function is thus

$$\psi_A = \psi_A^{\mathrm{SM}} \phi_{\mathrm{c.m.}}^{-1} = \left(\frac{A}{\pi b^2}\right)^{-3/4} b^{-3A/2} \exp\left[-\sum_i \frac{1}{2b^2}(\vec{r}_i - \vec{R})^2\right] \times \hat{A} \prod_{i=1}^{A} p_{\alpha_i}(\vec{r}_i/b), \tag{4.5}$$

where the antisymmetrizer $\hat{A}$ is defined so as to include the appropriate normalization factor, here $(A!)^{-1/2}$. Due to the antisymmetrization only the highest powers in the polynomials p_α contribute. This allows us to rewrite

$$\hat{A} \prod_{i=1}^{A} p_{\alpha_i}(\vec{r}_i/b) = \hat{A}' \prod_{i=1}^{A} p'_{\alpha_i}(\vec{r}'_i/b) = \frac{1}{\sqrt{A}} \sum_i (-1)^{A-i} p'_{\alpha_i}(\vec{r}'_A/b) \times \hat{A} \prod_{k}^{A-1} p'_{\alpha_{k'}}(\vec{r}'_k/b), \tag{4.6}$$

where

$$k' = \begin{cases} k, & k < i, \\ k+1, & k \geq i, \end{cases}$$

and

$$p'_\alpha(\vec{r}'/b) = \left(\frac{b'}{b}\right)^{m_\alpha} p_\alpha(\vec{r}'/b'). \tag{4.7}$$

Here the prime on $\hat{A}$ indicates antisymmetrization with respect to the coordinates $\vec{r}'_i = \vec{r}_i - \vec{R}'$ rather than $\vec{r}_i$ or $\vec{r}_i - \vec{R}$. In the last expression in (4.6) the $\hat{A}$ operates on the $A-1$ coordinates $\vec{r}'_i$, and the factor $A^{-1/2}$ results from the modification of the associated normalization constant. We thus obtain

$$\psi_A = \frac{1}{\sqrt{A}} \sum_{i=1}^{A} \phi_{\alpha_i}(\vec{r}'_A) \psi^{\alpha_i}_{A-1}(\vec{r}'_1 \cdots \vec{r}'_{A-1}), \tag{4.8}$$

with

$$\phi_\alpha(\vec{r}'_A) = b'^{-3/2} p_\alpha(\vec{r}'_A/b') \exp\left(-\frac{r'^2_A}{2b'^2}\right), \tag{4.9}$$

and

$$\psi^{\alpha_i}_{A-1}(\vec{r}'_1 \cdots \vec{r}'_{A-1}) = \left(\frac{A}{A-1}\right)^{m_{\alpha_i}/2} (-1)^{A-i} \times \tilde{\psi}^{\alpha_i}_{A-1}(\vec{r}'_1 \cdots \vec{r}'_{A-1}), \tag{4.10}$$

where

$$\tilde{\psi}^{\alpha_i}_{A-1}(\vec{r}'_1 \cdots \vec{r}'_{A-1}) = \left(\frac{A-1}{\pi b^2}\right)^{-3/4} b^{-3/2(A-1)} \times \exp\left(-\sum_k^{A-1} \frac{r'^2_k}{2b^2}\right) \hat{A} \prod_k^{A-1} p'_{\alpha_{k'}}(\vec{r}'_k/b). \tag{4.11}$$

It can easily be shown that the ψ^α_{A-1} are orthogonal.

The single-particle orbitals ϕ_α (4.9) thus play the role of the natural orbitals[12] with respect to the wave function ψ_A, i.e., they diagonalize the density matrix $S_{\alpha\beta}$ in the intrinsic frame:

$$S_{\alpha\beta} = \left(\frac{A}{A-1}\right)^{m_\alpha} \langle \tilde{\psi}^\alpha_{A-1} | \tilde{\psi}^\beta_{A-1} \rangle = S_\alpha \delta_{\alpha\beta}. \tag{4.12}$$

For nonspurious states, e.g. the hole in the highest occupied shell, only the highest powers of the polynomials, which are the same for $p'_\alpha(\vec{r}'_i/b)$ and $p_\alpha(\vec{r}_i/b)$, contribute and $\tilde{\psi}^\alpha_{A-1}$ is normalized to one [cf. (4.5)]. We thus find simply $S_\alpha = [A/(A-1)]^{m_\alpha}$.

For deeper shells $\langle \tilde{\psi}^\alpha_{A-1} | \tilde{\psi}^\alpha_{A-1} \rangle < 1$, where the reduction can be directly ascribed to the spuriosity of the shell model state. The explicit calculation of these norms is presented in Appendix A.

If we do not go beyond the $0p$ shell nuclei (for which nuclei the c.m. corrections are most significant) explicit calculations are not necessary, for the occupation probability of the $0s$ shell can be directly deduced from the spectroscopic sum rule (3.1). For example, for ^{12}C we find[13]

$$S_{0p} = \frac{A}{A-1} = \frac{12}{11}$$

and thus

$$S_{0s} = \tfrac{1}{4}(12 - 8 S_{0p}) = \frac{9}{11}.$$

In Appendix B we show that (3.1) is only one of a series of sum rules which allow one to very simply determine the occupation probabilities for heavier nuclei.

The presently available experimental information on knock-out reactions on light nuclei does not seem precise enough to really distinguish between the nontranslational invariant shell model prediction and the c.m. corrected values. Since relative spectroscopic factors can be measured more accurately it would be especially interesting to determine the ratios of the occupation probabilities of the various shells. Moreover, this tends to enhance the c.m. effects. For example, for ^{12}C the c.m. corrected value of $S_{0s}/S_{0p} = \frac{3}{4}$ instead of 1. Dynamical effects such as short-range correlations induced by the hard core in the two-nucleon interaction will also cause deviations from the shell model prediction, i.e., they lead to a depletion of the occupied shells, and therefore a reduction of the occupation probabilities. However, since the depletion factors have been shown[14] to be fairly independent of the shell, the relative occupation probabilities are not expected to be strongly affected by the short-range correlations.

In a similar way we obtain the c.m. corrections for the single-particle energies ϵ_α. Taking the expectation value of the kinetic energy one finds from (2.14)

$$\langle\psi_A|T|\psi_A\rangle-\frac{1}{S_\alpha}\langle\psi^\alpha_{A-1}|T|\psi^\alpha_{A-1}\rangle=\frac{A}{A-1}\left\langle\phi_\alpha\left|\frac{p^2}{2m}\right|\phi_\alpha\right\rangle=\tfrac{1}{2}e^{\mathrm{HO}}_\alpha, \tag{4.13}$$

and thus

$$\epsilon_\alpha=\tfrac{1}{2}e^{\mathrm{HO}}_\alpha+v_\alpha, \tag{4.14}$$

where

$$v_\alpha=\langle\psi_A|V|\psi_A\rangle-\frac{1}{S_\alpha}\langle\psi^\alpha_{A-1}|V|\psi^\alpha_{A-1}\rangle. \tag{4.15}$$

We thus find, in contrast with previous treatments of this problem, the contribution of the kinetic energy $\frac{1}{2}e^{\mathrm{HO}}_\alpha$ is the same as in the shell model frame.[15] Being purely relative the potential is also not directly affected by the c.m. motion. However, the spurious components of the shell model hole wave function correspond to internal configurations in which the hole is in a different, higher shell. Thus v_α as calculated in the shell model is actually a linear combination of the intrinsic v_α. This effect can be determined from the expansion of the shell model hole wave function (A9). Using the result of Appendix A we find

$$v^{\mathrm{SM}}_\alpha=N_\alpha v^{\mathrm{int}}_\alpha+\sum_{\beta,\,m_\beta>m_\alpha}(C^\beta_\alpha)^2N_\beta v^{\mathrm{int}}_\beta, \tag{4.16}$$

which can be inverted to determine the v^{int}_α from the v^{SM}_α. For example, the 20% spuriosity of the 0s state in ^{16}O implies that

$$v^{\mathrm{SM}}_{0s}=\tfrac{4}{5}v^{\mathrm{int}}_{0s}+\tfrac{1}{5}v^{\mathrm{int}}_{0p}. \tag{4.17}$$

Thus

$$v^{\mathrm{int}}_{0s}=\tfrac{5}{4}v^{\mathrm{SM}}_{0s}-\tfrac{1}{4}v^{\mathrm{SM}}_{0p}, \tag{4.18}$$

and

$$\epsilon^{\mathrm{int}}_{0s}=\epsilon^{\mathrm{SM}}_{0s}+\tfrac{1}{4}(v^{\mathrm{SM}}_{0s}-v^{\mathrm{SM}}_{0p}). \tag{4.19}$$

The c.m. correction thus increases the binding of the 0s shell. From the results of published HF calculations[9] we estimate this to be a 4–5 MeV effect in ^{16}O.

We note that no correction is necessary for the total contribution of the potential to the binding energy

$$\frac{1}{2}\sum_\alpha v^{\mathrm{SM}}_\alpha=\frac{1}{2}\sum_\alpha S_\alpha v^{\mathrm{int}}_\alpha, \tag{4.20}$$

as one would expect since V is purely relative. In this sense the modification of ϵ_α can be viewed as being necessary in order to cancel the effects of $S_\alpha\neq1$ when we go to the intrinsic frame.

In passing we note that the kinetic energy contribution to E_A in the intrinsic frame is, using (3.4), (3.5), (4.13), and (B10)

$$\frac{1}{4}\sum_\alpha S_\alpha e^{\mathrm{HO}}_\alpha+\tfrac{1}{2}(1-\eta)\sum_\alpha S_\alpha\left\langle\phi_\alpha\left|\frac{p^2}{2m}\right|\phi_\alpha\right\rangle=\frac{A-1}{2A}\sum_\alpha S_\alpha e^{\mathrm{HO}}_\alpha=\frac{1}{2}\sum_\alpha e^{\mathrm{HO}}_\alpha-\tfrac{3}{4}\omega, \tag{4.21}$$

which differs from the shell model result $\frac{1}{2}\sum e^{\mathrm{HO}}_\alpha$ by $\frac{3}{4}\omega$, the kinetic energy of the c.m. This is thus the only correction necessary for the calculation of the intrinsic energy.

As an illustration of the c.m. corrections derived above, it is instructive to consider the simple example of the $A=2$ nucleus built of identical nucleons. The shell model ground state configuration is (0s)(0p). One thus finds

$$S_{0p}=\frac{A}{A-1}=2,$$

and

$$S_{0s}=A-S_{0p}=0,$$

that is, the 0s hole state is completely spurious, i.e., does not exist. This reflects the fact that in the intrinsic frame both nucleons are actually in a relative p state. For the same reason one finds $v^{\mathrm{SM}}_{0s}=v^{\mathrm{SM}}_{0p}$.

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APPENDIX A

In order to calculate the norm of ψ^α_{A-1} we expand the corresponding shell model wave function

$\psi^{\alpha}_{A-1,\mathrm{SM}}$ in the eigenstates of c.m. motion $\phi_{\mathrm{c.m.}}$,

$$\psi^{\alpha}_{A-1,\mathrm{SM}} = \tilde{\psi}^{\alpha}_{A-1}\,\phi^{0s}_{\mathrm{c.m.}} + \sum_{\beta\neq 0s} \bar{\psi}^{\alpha}_{A-1,\beta}\,\phi^{\beta}_{\mathrm{c.m.}}\,. \tag{A1}$$

Since all the terms on the right-hand side are orthogonal we have

$$N_{\alpha} \equiv \langle \tilde{\psi}^{\alpha}_{A-1} | \tilde{\psi}^{\alpha}_{A-1}\rangle = 1 - \sum_{\beta\neq 0s} \langle \bar{\psi}^{\alpha}_{A-1,\beta}\,\phi^{\beta}_{\mathrm{c.m.}} | \bar{\psi}^{\alpha}_{A-1,\beta}\,\phi^{\beta}_{\mathrm{c.m.}}\rangle\,, \tag{A2}$$

where the last term is just the "spuriosity" of the shell model hole state.

To develop the expansion (A1) we use the explicit form of $\tilde{\psi}^{\alpha}_{A-1}$ (4.11). We first consider the one-dimensional problem for identical particles. Setting $b=1$ for simplicity, we have

$$\psi^{\alpha_i}_{\mathrm{NS}} \equiv \tilde{\psi}^{\alpha_i}_{A-1}\,\phi^{0s}_{\mathrm{c.m.}} = \hat{A}\prod_{k=1}^{A-1} \pi^{-1/4} h'_{\alpha_{k'}}(r_k - R')\exp(-\tfrac{1}{2}r_k^{\,2}), \tag{A3}$$

where

$$k' = \begin{cases} k, & k<i\,,\\ k+1, & k\geq i\,,\end{cases}$$

and thus

$$\begin{aligned}\psi^{\alpha}_{\mathrm{NS}} &= \psi^{\alpha}_{A-1,\mathrm{SM}} + \sum_{\beta>\alpha} C^{\beta}_{\alpha}\psi^{\beta}_{A-1,\mathrm{SM}} h_{\beta-\alpha}(R'\sqrt{A-1}) + \sum_{\gamma>\beta>\alpha} C^{\beta}_{\alpha}C^{\gamma}_{\beta}\psi^{\gamma}_{A-1,\mathrm{SM}} h_{\beta-\alpha}(R'\sqrt{A-1})h_{\gamma-\beta}(R'\sqrt{A-1}) + \cdots\\ &= \psi^{\alpha}_{A-1,\mathrm{SM}} + \sum_{\beta>\alpha} C^{\beta}_{\alpha}h_{\beta-\alpha}(R'\sqrt{A-1})\Big[\psi^{\beta}_{A-1,\mathrm{SM}} + \sum_{\gamma>\beta} C^{\gamma}_{\beta}\psi^{\gamma}_{A-1,\mathrm{SM}} h_{\gamma-\beta}(R'\sqrt{A-1}) + \cdots\Big]\\ &= \psi^{\alpha}_{A-1,\mathrm{SM}} + \sum_{\beta>\alpha} C^{\beta}_{\alpha}\psi^{\beta}_{\mathrm{NS}} h_{\beta-\alpha}(R'\sqrt{A-1})\,,\end{aligned} \tag{A9}$$

where we have used the fact that $C^{\alpha}_{\alpha}=-1$. Since

$$\phi^{\beta}_{\mathrm{c.m.}} = h_{\beta}(R'\sqrt{A-1})\,\phi^{0s}_{\mathrm{c.m.}} \tag{A10}$$

is normalized to one, the polynomials $h_{\beta}(R'\sqrt{A-1})$ do not modify the normalization of the terms on the right-hand side of (A9). We thus find

$$N_{\alpha} = \langle \psi^{\alpha}_{\mathrm{NS}} | \psi^{\alpha}_{\mathrm{NS}}\rangle = 1 - \sum_{\beta>\alpha} (C^{\beta}_{\alpha})^2 N_{\beta}\,. \tag{A11}$$

The extension to three dimensions is accomplished by replacing α by the set $(\alpha_x,\alpha_y,\alpha_z)$, and C^{β}_{α} by $C^{\beta_x}_{\alpha_x}, C^{\beta_y}_{\alpha_y}, C^{\beta_z}_{\alpha_z}$. The only modification necessary to include the spin-isospin degree of freedom is to restrict the sum over the states to the same spin and isospin as α.

Applying this method to ^{16}O and ^{40}Ca we find using (4.12) for ^{16}O

$$N_{0p} = 1, \quad S_{0p} = \frac{A}{A-1} = \frac{16}{15},$$

and

$$h'_{\alpha}(r) = \frac{1}{(\alpha!\,2^{\alpha})^{1/2}}\left(\frac{A}{A-1}\right)^{\alpha/2} H_{\alpha}\left[r\left(\frac{A-1}{A}\right)^{1/2}\right], \tag{A4}$$

where H_{α} denotes the Hermite polynomial. The corresponding shell model wave function is

$$\psi^{\alpha_i}_{A-1,\mathrm{SM}} = \hat{A}\prod_{k=1}^{A-1} \pi^{-1/4} h_{\alpha_{k'}}(r_k)\exp(-\tfrac{1}{2}r_k^{\,2}), \tag{A5}$$

with

$$h_{\alpha}(r) = \frac{1}{(\alpha!\,2^{\alpha})^{1/2}}\,H_{\alpha}(r) \tag{A6}$$

Using the addition theorem[16] for Hermite polynomials we find

$$h'_{\alpha}(r-R') = -\sum_{\beta\leq\alpha} (-1)^{\alpha-\beta} C^{\alpha}_{\beta}\, h_{\beta}(r)\, h_{\alpha-\beta}(R'\sqrt{A-1})\,, \tag{A7}$$

with

$$C^{\alpha}_{\beta} = -(A-1)^{(\beta-\alpha)/2}\left(\frac{\alpha!}{\beta!\,(\alpha-\beta)!}\right)^{1/2}, \tag{A8}$$

$$N_{0s} = 1 - 3(C^1_0)^2 N_{0p} = 1 - \frac{3}{A-1}, \quad S_{0s} = N_{0s} = \frac{4}{5},$$

and for ^{40}Ca

$$N_{0d} = N_{1s} = 1, \quad S_{0d} = S_{1s} = \left(\frac{A}{A-1}\right)^2 = \frac{1600}{1521},$$

$$N_{0p} = 1 - [\,(C^2_1)^2 + 2(C^1_0)^2\,]\,N_{0d} = 1 - \frac{4}{A-1},$$

$$S_{0p} = \frac{A}{A-1}\,N_{0p} = \frac{1400}{1521},$$

$$N_{0s} = 1 - 3(C^1_0)^2 N_{0p} - [\,3(C^2_0)^2 + 3(C^1_0)^4\,]\,N_{0d} = 1 - \frac{3}{A-1}\left(1 - \frac{4}{A-1}\right) - \frac{6}{(A-1)^2},$$

$$S_{0s} = N_{0s} = \frac{1410}{1521}.$$

APPENDIX B

In this Appendix we present a second method for obtaining the occupation probabilities. We define the raising and lowering operators for the intrinsic HO wave function as

$$\vec{a}^{\dagger} = \frac{1}{\sqrt{2}}\left[\frac{\vec{r}_A - \vec{R}'}{b'} - b'\left(\vec{\partial}_A - \frac{1}{A}\vec{\partial}_{\vec{R}}\right)\right],$$

and

$$\vec{a} = \frac{1}{\sqrt{2}}\left[\frac{\vec{r}_A - \vec{R}'}{b'} + b'\left(\vec{\partial}_A - \frac{1}{A}\vec{\partial}_{\vec{R}}\right)\right], \tag{B1}$$

which satisfy the commutation relation

$$[a_i, a_j^{\dagger}] = \delta_{ij} \qquad (i = x, y, z), \tag{B2}$$

and thus

$$\vec{a}^{\dagger}\cdot\vec{a}\,\phi_\alpha(\vec{r}'_A) = m_\alpha \phi_\alpha(\vec{r}'_A). \tag{B3}$$

Applying $\vec{a}^{\dagger}\cdot\vec{a}$ to the internal wave function (4.8) we find

$$\vec{a}^{\dagger}\cdot\vec{a}\,\psi_A = \frac{1}{\sqrt{A}}\sum_\alpha m_\alpha \phi_\alpha(\vec{r}'_A)\psi^\alpha_{A-1}, \tag{B4}$$

and thus

$$A\langle\psi_A|\vec{a}^{\dagger}\cdot\vec{a}\,|\psi_A\rangle = \sum_\alpha m_\alpha \langle\psi^\alpha_{A-1}|\psi^\alpha_{A-1}\rangle = \sum_\alpha m_\alpha S_\alpha. \tag{B5}$$

The left-hand side of (B5) can also be constructed in another way. Noting that the operators $\vec{a}^{\dagger}, \vec{a}$ are purely relative, we multiply ψ_A by $\phi^{\rm os}_{\rm SM}$ and return to the shell model wave function. The intrinsic operators (B1) can be expressed in terms of their shell model and c.m. counterparts:

$$\vec{a}^{(\dagger)} = \left(\frac{A}{A-1}\right)^{1/2}\left(\vec{a}^{(\dagger)}_{\rm SM} - \frac{1}{A}\vec{a}^{(\dagger)}_{\rm c.m.}\right), \tag{B6}$$

where

$$\vec{a}^{(\dagger)}_{\rm SM} = \frac{1}{\sqrt{2}}\left(\frac{\vec{r}_A}{b} \pm b\,\vec{\partial}_A\right), \tag{B7}$$

$$\vec{a}^{(\dagger)}_{\rm c.m.} = \frac{1}{\sqrt{2}}\left(\sqrt{A}\,\frac{\vec{R}}{b} \pm \frac{b}{\sqrt{A}}\vec{\partial}_{\vec{R}}\right). \tag{B8}$$

Since $\psi^{\rm SM}_A$ represents the ground state, $\vec{a}_{\rm c.m.}|\psi^{\rm SM}_A\rangle = 0$; and thus

$$A\langle\psi_A|\vec{a}^{\dagger}\cdot\vec{a}\,|\psi_A\rangle = \frac{A^2}{A-1}\langle\psi^{\rm SM}_A|\vec{a}^{\dagger}_{\rm SM}\cdot\vec{a}_{\rm SM}|\psi^{\rm SM}_A\rangle = \frac{A}{A-1}\sum_\alpha m_\alpha, \tag{B9}$$

which gives the sum rule

$$\sum_\alpha m_\alpha\left(S_\alpha - \frac{A}{A-1}\right) = 0. \tag{B10}$$

By following the same procedure with the normal ordered operator

$$N[(\vec{a}^{\dagger}\cdot\vec{a})^p], \tag{B11}$$

one finds the generalized sum rule

$$\sum_\alpha \frac{m_\alpha!}{(m_\alpha - p)!}\left[S_\alpha - \left(\frac{A}{A-1}\right)^p\right] = 0. \tag{B12}$$

For $p = 0$ this reduces to the spectroscopic sum rule (3.1).

Setting $p = m_\alpha$ for the last shell (B12) immediately gives $S_\alpha = [A/(A-1)]^{m_\alpha}$ in agreement with the result obtained in Sec. 4. By decreasing p by steps of 1 the S_α for the inner shells can be successively determined.

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$$\langle\psi_A|T^A_{\rm c.m.}|\psi_A\rangle - \tfrac{1}{S_\alpha}\langle\psi^\alpha_{A-1}|T^{A-1}_{\rm c.m.}|\psi^\alpha_{A-1}\rangle = \tfrac{3}{4}\omega - \tfrac{3}{4}\omega = 0.$$

In the methods proposed in Refs. 8 (method II) and 9 and in the work of H. C. Lee and R. Y. Cusson [Ann. Phys. (N. Y.) 72, 353 (1972)], the explicit dependence of $T_{\rm c.m.}$ on A, which is necessary to obtain such a cancellation, was neglected.

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