We continue the investigations of the $^{16}$O ground state using the coupled-cluster expansion [exp($S$)] method with realistic nuclear interaction. In this stage of the project, we take into account the three nucleon interaction, and examine in some detail the definition of the internal Hamiltonian, thus trying to correct for the center-of-mass motion. We show that this may result in a better separation of the internal and center-of-mass degrees of freedom in the many-body nuclear wave function. The resulting ground state wave function is used to calculate the “theoretical” charge form factor and charge density. Using the “theoretical” charge density, we generate the charge form factor in the DWBA picture, which is then compared with the available experimental data. The longitudinal response function in inclusive electron scattering for $^{16}$O is also computed.

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I. INTRODUCTION

The coupled-cluster expansion, also called the exp($S$) method, was developed about 40 years ago by Coester [1]. It was then applied to finite nuclei quite successfully by Kümmerl and the Bochum group [2] using a representation of the wave function in coordinate space together with common interactions of that time. While the method in general is viewed as essentially exact, approximations are introduced stemming from truncations in the coupled cluster equations, as well as truncations in the model space. The results for the binding energy were well above the Coester-line and were taken as evidence for the presence of three-nucleon and higher order interactions.

While few further developments took place since that time, the ongoing expansion in computer power as well as the availability of more sophisticated nucleon-nucleon interactions suggests that one should go back to these precise methods. During the past several years we have reexamined the coupled cluster approach and applied it to the spherical nucleus $^{16}$O using the Argonne v18 potential [3]. We combine the mean field approach together with the coupled cluster expansion in a harmonic oscillator basis of $50 \ h \omega$ (which constitutes our truncated Hilbert space) and going up to the level of $4p4h$ clusters.

Further, we have expanded the formulation to include the Urbana IX three-nucleon interaction. The results are in reasonable agreement with the experiment and make the subject of the present paper. These results obtained using the coupled cluster expansion should be directly comparable with those obtained using the Variational Monte Carlo (VMC) [4] or the Green’s Function Monte Carlo (GFMC) methods, using the same interaction. Especially the GFMC method with the Argonne v18 potential and the Urbana IX three-nucleon interaction has proved quite accurate in nuclei with $A \leq 7$ [5], even though a certain uncertainty in the three-nucleon interaction model is responsible for a systematic lack of binding in the heavier systems. These difficulties will be addressed however in the future, by considering more sophisticated three-body interaction models.

In section II we briefly review the coupled-cluster approach as outlined in [3] when the Hamiltonian includes only the two-body interaction. We continue this discussion in section III with comments pertaining to the inclusion of the center-of-mass Hamiltonian, which is supposed to constrain the center-of-mass degrees of motion in the ground state wave function. In section IV we outline the changes necessary in order to include the three-nucleon interaction via a density-dependent approximation. In section V we show various observables calculated in the ground state for $^{16}$O. Finally, in section VI we present our conclusions and a brief outlook.

II. COUPLED-CLUSTER METHOD: A REVIEW

For a spherically symmetric nuclear system, consisting of both protons and neutrons, the total Hamiltonian is given as the sum of a nonrelativistic one-body kinetic energy, a two-nucleon potential and a three-nucleon potential.
\[ H = \sum_i T_i + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}^{\text{int}}. \] (2.1)

Since our calculation is carried out in configuration space, we need the nuclear interaction projected out in an operator format allowing for calculation of two- and three-body matrix elements. We chose to use the operator format of the Argonne and Urbana family potentials. The Argonne v18 model [6] is one of a new class of N N potentials that accurately fit both \( pp \) and \( nn \) scattering data up to 350 MeV with a \( \chi^2 / \text{datum} \) near one. The Urbana IX potential [7] includes a long-range two-pion exchange and a short-range phenomenological component. The strength of nuclear correlations.

III. CENTER-OF-MASS HAMILTONIAN

The correlated ground-state \(|0\rangle\) is a function of \( A \) sets of coordinates \( \{ \hat{r}_k, k = 1 \ldots A \} \). Consequently, the ground state wave function is not translationally invariant. As a result, it is common practice [3] to attempt solving the Schrödinger equation for the ground state of the internal Hamiltonian

\[ H_{\text{int}} = H - T_{\text{CM}}, \]

instead of the Hamiltonian (2.1). The internal Hamiltonian is entirely written in the center-of-mass frame by removing the center-of-mass kinetic energy, \( T_{\text{CM}} = P_{\text{CM}}^2 / (2 m) \), with \( m \) being the nucleon mass. Both the two- and three-nucleon interactions are given in terms of the relative distances between nucleons, so in this respect no corrections are needed.

However, this does not prevent the contamination of the correlated ground-state \(|0\rangle\) by the center-of-mass motion. Especially since we are interested in the calculation of the excited states spectrum, this contamination will result in spurious excitations of the center-of-mass. Moreover, the calculation of observables to be compared with experimental data which are taken in the center-of-mass frame, requires the evaluation of a many-body expansion as explained in [8]. This in turn relies on the assumption that we can neglect the correlations between the internal and center-of-mass degrees of freedom at the level of the correlated ground-state \(|0\rangle\). In order to ensure such a separation, a supplemental center-of-mass Hamiltonian is added

\[ H_{\text{CM}} = \beta_{\text{CM}} \left[ T_{\text{CM}} + \frac{1}{2} (m) \, \Omega^2 \, R_{\text{CM}}^2 \right]. \]

The center-of-mass Hamiltonian has the role of constraining the center-of-mass component of the ground state wave function [9]. Then, we have to identify a domain of values for the parameters \( \beta_{\text{CM}} \) and \( \Omega^2 \) such that the binding energy

\[ E = \langle H_{\text{int}} + H_{\text{CM}} \rangle - \langle H_{\text{CM}} \rangle \]

is insensitive to the choice of these parameters.

For the purpose of this analysis we leave out the three-nucleon interaction, and show results when including only the v18 \( NN \) interaction. Figures 1 and 2 show the \( \beta_{\text{CM}} \) dependence of center-of-mass and binding energies, respectively.

IV. THREE-NUCLEON INTERACTION CORRECTIONS

We will present here the corrections necessary to take into account the three-nucleon interaction as part of the
general nuclear interaction. As discussed before we consider the three-nucleon interaction as the sum of two components: a long-range two-pion exchange and a short-range phenomenological component. The calculation of the three-nucleon interaction has been presented elsewhere [10].

Given the form (2.1) of the Hamiltonian, we write the operator \( V_{\text{tri}} \) in second quantization as

\[
V_{\text{tri}} = \sum_{a_1 b_1 c_1 a_2 b_2 c_2} V_{a_1 b_1 c_1, a_2 b_2 c_2} a_{a_1}^\dagger a_{b_1}^\dagger a_{c_1} a_{a_2} a_{b_2} a_{c_2} .
\] (4.1)

Here, the matrix elements are given as integrals involving the single particle states (including spins)

\[
V_{a_1 b_1 c_1, a_2 b_2 c_2} = \langle \phi_{a_1} | \phi_{b_1} (2) \phi_{c_1} (3) | V_{\text{tri}} | \phi_{a_2} (1) \phi_{b_2} (2) \phi_{c_2} (3) \rangle .
\] (4.2)

In addition to being symmetric with respect to the interchange of the particles labelled 2 and 3

\[
V_{a_1 b_1 c_1, a_2 b_2 c_2} = V_{a_1 c_1 b_1, a_2 c_2 b_2} ,
\] (4.3)

the integrals (4.2) also satisfy the symmetry

\[
V_{a_1 b_1 c_1, a_2 b_2 c_2} = V_{c_1 a_1 b_1, c_2 a_2 b_2} .
\] (4.4)

The last property is a consequence of the cyclic sums involved in the definition of the interaction, which make the interaction invariant with respect to the labelling of the particles.

In previous applications the approximation has been made that such an interaction can be represented by a density dependent two-body interaction. While such a substitution is the easiest modification, it has been stated that this is insufficient [7]. However, the rigorous inclusion of the three-nucleon interaction in configuration space using the coupled-cluster method is seriously hampere...
We notice that only the first two terms in Eq. (4.10) have the form (4.5). However, in this particular case, it is a simple endeavor to calculate the missing third matrix element. We find that the magnitude of this term is small compared to the sum of the terms (4.5).

Second order contributions are calculated exactly as

\[
0 \langle S_2 | V | 0 \rangle = \frac{1}{4} \sum_{p_1 \neq p_2 h_1 h_2} S_{p_1 h_1, p_2 h_2} V_{tni, den}^{t p_1 h_1, p_2 h_2; p_1 h_1}.
\] (4.11)

At the present time, the third order corrections have not been evaluated. Their magnitude is expected to be small, and their inclusion is definitely next-order in terms of the present expansion.

### B. Mean Field Corrections.

In our approach to the coupled cluster formalism, the single particle orbits are eigenfunctions of an mean-field Hamiltonian, defined as the sum of a one-body kinetic energy term and a one-body mean-field potential. The later is not unique, and in the maximum overlap hypothesis \( S_1 = 0 \), the mean-field is defined as

\[
0 \langle U_0 | 1p1h \rangle = 0 \left\{ V + [S_2, V] + [S_3, V] \right\} | 1p1h \rangle.
\] (4.12)

Correspondingly, the contributions due to the three-nucleon interaction can be written as the sum of three terms

\[
0 \langle V_{tni} a_j^\dagger a_i a_k | 0 \rangle
+ 0 \langle [S_2, V_{tni}] a_j^\dagger a_i a_k | 0 \rangle
+ 0 \langle [S_3, V_{tni}] a_j^\dagger a_i a_k | 0 \rangle.
\] (4.13)

In leading order, the three-nucleon interaction correction of the mean-field is given as

\[
0 \langle V_{tni} a_j^\dagger a_i a_k | 0 \rangle = \frac{1}{2} \sum_{h_1 h_2} \left\{ V_{h_1 h_2 h_1 h_2 p} - V_{h_2 h_1 h_2 h_1 p} + V_{h_1 h_2 h_2 p h_1} - V_{h_1 h_2 h_1 p h_2} + V_{h_2 h_1 h_1 h_2 p} - V_{h_1 h_2 h_2 h_1 p} \right\}.
\] (4.14)

Again, using the symmetries (4.3, 4.4), Eq. (4.14) becomes

\[
0 \langle V_{tni} a_j^\dagger a_i a_k | 0 \rangle = \sum_{h_1 h_2} \left\{ \frac{1}{2} V_{h_1 h_2 h_1 h_2 p} - V_{h_1 h_2 h_2 h_1 p} + V_{h_1 h_2 h_2 p h_1} - \frac{1}{2} V_{h_1 h_2 h_2 h_1 p} \right\}.
\] (4.15)

The second- and third-order contributions in Eq. (4.13) look very similar when one uses the proposed reduction of the three-body force, Eq. (4.7), for the account of the 3p3h correlations. Then, by making use of the full antisymmetry of \( S_2 \) and \( V_{tni, den} \) we can show that the required corrections can be written as

\[
\sum_{p_1 \neq p_2 h_1 h_2} \left\{ \left( V_{h_1 p_2 p_1 h_2} - 2 V_{h_1 p_2 p_2 h_2} - 2 V_{h_2 h_1 h_2 p_1 p_2} \right) \epsilon_{ph} + \epsilon_{p_1 h_1} + \epsilon_{p_2 h_2} \right\}.
\] (4.16)

To maintain the symmetry we have also added similar terms to the \( hh \)- and \( pp \)-terms of the single particle Hamiltonian.

### V. OBSERVABLES

The results we report here are carried out in a 50\( h_\omega \) configuration space. In general, the expectation value of any arbitrary operator \( A \) in the correlated ground-state \(| 0 \rangle \) is obtained as

\[
\hat{a} = \langle 0 | e^S A e^{-S} \hat{S}^\dagger | 0 \rangle,
\]

where similarly to the cluster correlation operator \( S^\dagger \), the new operator \( \hat{S}^\dagger \) is expanded out in terms of \( ph \)-creation operators

\[
\hat{S}^\dagger = \sum_n \frac{1}{n!} \tilde{S}_n \hat{O}_n^\dagger.
\]

The amplitudes \( \tilde{S}_n \) are calculated iteratively in terms of the \( S_n \) amplitudes [3].

The resulting binding energy and charge radii for the Argonne \( v18 \) with/without the Urbana IX potential, are shown in Table I. Note that the charge radii correspond to the “theoretical” charge density as explained below. The calculation is shown to be stable with respect to the two cut-off parameters, \( l_{max} \) and \( n_{max} \), which control the size of the configuration space as \( N_{max} = 2n_{max} + l_{max} \). Figure 3 shows the binding energy for \( ^{16}O \) calculated using the \( v18 \) and Urbana IX interactions, as a function of the \( (l_{max}, n_{max}) \) cut-off pair, and show the calculation to be reasonably converged for \( l_{max} = 11, 12 \) and \( n_{max} = 22, 25 \), same as the \( v18 \) based calculation of [3].

### A. Charge Form Factor

The charge form factor is calculated as the sum of a one- and two-body operator. The one-body component is evaluated in the nonrelativistic one-body Born-approximation picture, where the charge form factor is given as
\[ F_L(q) = \langle \bar{0} | \sum_k f_k(q^2) e^{i\vec{q} \cdot \vec{r}_k} | \bar{0} \rangle. \]

Here \( f_k(q^2) \) is the nucleon form factor, which takes into account the finite size of the nucleon \( k \). In our calculation we use the Iachello-Jackson-Lande [12] nucleon-form factors. Note however that at the rather small values of \( q \) involved in the present discussion, \( q < 4 \) fm\(^{-1} \), the differences between the various models of the nucleon form factor are expected to be small [13].

As seen from previous calculations [4], the main contributions from the two-body charge density not related to center-of-mass corrections is expected to come from the the \( \pi \) - and \( \rho \)-exchange “seagull” diagrams. These are taken into account as referred in the model-independent part of the “Helsinki meson-exchange model” [13]. In this model the pions and \( \rho \)-meson propagators are replaced by the Fourier transforms of the isospin dependent spin-spin and tensor components of the \( \pi \) and \( \rho \) part of the “Helsinki meson-exchange model” [13]. In this model the pion and \( \rho \)-meson propagators are replaced by the Fourier transforms of the isospin dependent spin-spin and tensor components.

In Eq. (5.1), the longitudinal-longitudinal distribution function \( \rho_{LL}(q) \) is given in terms of the proton-proton two-body density as

\[ \rho_{LL}(q) = \int d\vec{r}_1 \int d\vec{r}_2 \, j_0(q|\vec{r}_1 - \vec{r}_2|) \rho^{(p,p)}(\vec{r}_1, \vec{r}_2) \cdot \]

where \( \rho(q) \) is the nuclear charge operator

\[ \rho(q) = \frac{1}{2} \sum_{i=1}^{A} e^{i\vec{q} \cdot \vec{r}_i} (1 + \tau_{z,i}) \cdot \]

In Eq. (5.1), the longitudinal-longitudinal distribution function \( \rho_{LL}(q) \) is given in terms of the proton-proton two-body density as

\[ \rho_{LL}(q) = \int d\vec{r}_1 \int d\vec{r}_2 \, j_0(q|\vec{r}_1 - \vec{r}_2|) \rho^{(p,p)}(\vec{r}_1, \vec{r}_2) \cdot \]

We have outlined recently [3] the calculation of the proton-proton two-body density in the coupled-cluster framework, as the expectation value

\[ \rho^{(p,p)}(\vec{r}_1, \vec{r}_2) = \frac{1}{4} \sum_{i,j} \langle \bar{0} | \delta(\vec{r}_1 - \vec{r}_i)\delta(\vec{r}_2 - \vec{r}_j)(1 + \tau_{z,i})(1 + \tau_{z,j})|\bar{0} \rangle \cdot \]
with the normalization
\[
\int d\vec{r}_1 \int d\vec{r}_2 \rho^{(p-p)}(\vec{r}_1, \vec{r}_2) = Z - 1.
\] (5.5)

Figure 7 depicts the results of the present calculation for $^{16}\text{O}$. Again, the theoretical calculation corresponds to the $\epsilon \Lambda + \chi^2 + H_{CM}$ interaction in Table I. Since no experimental data are available for $^{18}\text{O}$ we compare these results with the $^{12}\text{C}$ experimental data of [19], where an estimate [20] for contributions from large $\omega$ has been added. Preliminary theoretical results for $^{12}\text{C}$ obtained using the coupled-cluster method have been recently reported in [21] and shown to be close to the $^{16}\text{O}$ result. The large error bars on the experimental data are largely due to systematic uncertainties associated with tail contribution [22].

VI. CONCLUSIONS AND OUTLOOK

The goal of our effort is to make a contribution to the ongoing effort of building realistic models of nuclear structure that explicitly account for realistic correlations. In a first stage we focus our attention on obtaining a realistic description for the ground state of a doubly-magic nucleus using the coupled-cluster method. In this sense, the present calculation represents the most detailed calculation available today, using the coupled-cluster method for a nuclear system with $A > 8$. We base our calculation on what is considered the best realistic description of the two- and three-body interactions available today [5].

At this stage we have proved conclusively that it is possible to choose a large enough configuration space to handle the relatively hard-core of the nucleon-nucleon interaction. We believe that we have also identified the dominant contributions of the three body interaction, and we have introduced an effective two-body interaction, accordingly.

An interesting conclusion from the charge form factor calculation has to do with the importance of the distortion effect due to the interaction between the electron and the Coulomb field of the nucleus. In this context we have shown that it is desirable to compare the distorted charge form factor with the experimental one, and to de-emphasize the comparisons regarding the nuclear charge density, which is not very surprising as the charge form factor represents the primary result of the experiment.

In this paper we have confined ourselves to presenting a purely nonrelativistic description of the charge form factor in $^{16}\text{O}$. In the future it will be interesting to get a better understanding of the importance of relativistic effects on the charge form factor calculation. In this sense we plan to redo this calculation using the relativistic description of the one-body charge form factor of [16], together with a consistent relativistic derivation of the two-body meson-exchange density [23].

With the calculation of the $^{16}\text{O}$ ground state completed we intend to extend our formulation to address the calculation of discrete excited states as well as neighboring odd-even nuclei. This is a necessary step in the quest of modeling the (e,e'N) reaction, where the final state has the asymptotic form of a distorted wave times a discrete state of the $(A-1)$ nucleus. However, this is not a solution to the Hamiltonian close to the origin, and thus the wave function needs to be modified in the region of the origin.

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TABLE I. Energy expectation values and theoretical charge radii for $^{16}$O.

<table>
<thead>
<tr>
<th>Interaction</th>
<th>B.E. [MeV/nucleon]</th>
<th>r.m.s [fm$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_{18}$</td>
<td>-5.9</td>
<td>2.85</td>
</tr>
<tr>
<td>$v_{18} +$UIX</td>
<td>-7.7</td>
<td>2.74</td>
</tr>
<tr>
<td>$v_{18} +$UIX + $H_{CM}$</td>
<td>-8.0</td>
<td>2.62</td>
</tr>
<tr>
<td>expt.</td>
<td>8.00</td>
<td>2.73 ± 0.025</td>
</tr>
</tbody>
</table>
FIG. 1. $\beta_{CM}$ dependence of center-of-mass energy (using $v_{18}$).

FIG. 2. $\beta_{CM}$ dependence of binding energy (using $v_{18}$).

FIG. 3. $(l_{\text{max}}, n_{\text{max}})$ cut-off dependence of binding energy (using $v_{18}$ and UIX).

FIG. 4. Charge form factors for $^{16}\text{O}$, using the Argonne $v_{18}$ and Urbana IX potentials.

FIG. 5. Charge density for $^{16}\text{O}$, including meson exchange contributions.

FIG. 6. Charge form factor for $^{16}\text{O}$, obtained in the DWBA picture ($v_{18} + \text{UIX} + \text{ME}$).
FIG. 7. Coulomb sum for $^{16}$O, compared with “experimental” $^{12}$C data which include theoretically determined high-energy tail corrections.