Translationally Invariant Local Densities for Light Nuclei from No-Core-Shell-Model Calculations

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This thesis titled
Translationally Invariant Local Densities for Light Nuclei from No-Core-Shell-Model
Calculations

by

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the Department of Physics and Astronomy
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Applications of No-Core-Shell-Model (NCSM) densities in reaction calculations require that they are translationally invariant. In order to obtain translationally invariant local one-body densities for $^4$He, $^6$He, and $^6$Li we first reconstruct them in a space-fixed, coordinate-space frame from the output of NCSM calculations. We study their shapes in coordinate as well as momentum space as function of the size of the basis employed. The center-of-mass contribution is exactly removed in the momentum space representation. Form factors and RMS radii are computed from the translationally invariant local density.
This work is dedicated to my friends and family that believed in me even when I didn’t believe in myself.
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4.8 The proton t.i. local density $\rho^{(K)}(r)C_{K}$ and $\rho^{(K)}(q)C_{K}$ of the excited state, $3^+$, for $^6$Li ($N_{\text{max}} = 14$). Panel (a) shows the coordinate space density with $\rho^{(2)}(r)$ multiplied by a factor of 5, while panel (b) depicts the momentum space density with $\rho^{(0)}(q)$ multiplied by $Y_0^0(\hat{q})$ and $\rho^{(2)}(q)$ is multiplied by a factor of 5.

C.1 Coordinate space representation of the one-body local density $\rho^{(0)}_{sf}(r)$, for $^6$He in the ground state as a function of $r^2$.

C.2 Momentum space representation of the one-body local density $\rho^{(0)}_{sf}(q) \times Y_0^0(\hat{q})$, for $^6$He in the ground state after a single Fourier transform as a function of $q^2$.

C.3 Coordinate space representation of the one-body local density $\rho^{(0)}_{ti}(r)$, for $^6$He in the ground state after the removal of the c.m. and Fourier transform to coordinate space as a function of $r^2$.

C.4 The momentum space one-body local density $\rho^{(0)}_{sf}(q)$, for $^6$He in the ground state as a function of $q^2$. Grid points between different subsections of the coordinate space local density are changed from 800 to 50.

C.5 Fourier transformation integral values for $4\pi \rho(r) \rho(q)$ for five different values of $q$ as function of $r$. The values of $q$ are given in the legends.
1 Introduction and Motivation

Interpreting and calculating weakly bound, light nuclei as quantum halo systems is a problem of long-standing interest [1]. In this context $^6$He can be understood as prototypical two-neutron halo system, where the tightly bound subsystem (here the $\alpha$-particle) is taken as an elementary degree of freedom, and the neutrons are weakly bound. Their binding is provided by inter-cluster interactions. This picture of a halo nucleus lead to the development of a variety of few-body methods [2, 3]. The small binding energies of those light halo nuclei and their corresponding extended spatial structure make them also good candidates for study within effective theories, in which the momentum transfer is sufficiently small so that the interior structure of the core is not resolved. In Refs. [4, 5] this was worked out for the case of an $\alpha$-particle core.

A different picture of this structure is obtained in reactions of halo-nuclei with proton targets as carried out at the Rikagaku Kenkyusho Institute of Physical and Chemical Research (RIKEN) for $^6$He and $^8$He at higher energies in inverse kinematics [6–9]. High energy, proton-induced reactions are well suited for studying halo degrees of freedom, since high energies allow rapid transfer from initial to final state. Here, the instantaneous structure is probed, since the time-scale of the halo motion is much longer than the reaction process. Since excited few-body halo states are quite fragile, it is useful to focus on elastic scattering which provides information about the spatial extension of the halo. Already over a decade ago, rare isotope (RI) beams were used at the Helmholtz Centre for Heavy Ion Research (GSI) and RIKEN to study the cross sections for proton-nucleus scattering in inverse kinematics and extract nuclear sizes. At these energies optical models are an appropriate tool to provide insight into the dynamics. Optical potentials are potentials with imaginary components which effectively account for internal excitations of the nucleus or its breakup, which are inelastic scattering processes. Beam particles involved in inelastic processes lose energy and thus are no longer part of the elastic channel, which requires energy conservation. They are considered "absorbed" as light is
in an opaque medium. Therefore, nuclear potentials that allow for absorption from the elastic channel are often called optical potentials. Analysis of reaction data using such models showed the existence of a halo but lacked sufficient precision to pin down nuclear radii accurately. In the case of $^6$He and $^8$He subsequent measurements of the nuclear charge radii via atomic isotope shifts [10, 11] are orders of magnitude more precise.

To gain information about the spin structure in halo nuclei, polarization observables have to be measured. In 2005, RIKEN set up the first experiment to extract such information, measuring the analyzing power $A_y$ in elastic scattering of $^6$He [6–8] from a proton target at 71 MeV/u. The results are surprising: the data disagreed with all available optical-model predictions, which nevertheless describe the differential cross section at this energy reasonably well [12, 13]. This apparent ‘$A_y$-problem’ suggests that folding models of the optical potential which are adequate in describing proton-nucleus scattering from stable nuclei are insufficient for reactions with halo nuclei. The obvious difference is the nuclear structure that enters the folding models.

Typical stable nuclei for which folding models are very successful are mostly spherical and have closed (filled) shells. Despite the ground state of $^6$He carrying the quantum number $0^+$, $^6$He is not a closed shell nucleus. Traditionally, microscopic optical potentials are constructed for closed shell nuclei by folding nucleon-nucleon (NN) amplitudes with the single-particle density matrix of the nucleus under consideration, see e.g. Ref. [14]. For a closed shell nucleus it can be shown analytically that only the central and spin-orbit parts of the NN transition matrix enters into the optical potential [15]. However, this is not true for nuclei with partially filled outer shells like $^6$He. The first extension for microscopic folding models beyond closed-shell nuclei was pioneered in Ref. [16]. However, the one-body density matrix employed there only could give a proof of principle, but was too simplistic to produce realistic calculations. On the other hand, that work paved the road for introducing state-of-the-art $ab$ $initio$ no-core-shell-model (NCSM) densities to scattering calculations based on optical potentials. Specifically, for
harmonic oscillator wave functions, which constitute the basis states for the NCSM, translationally invariant one-body densities can be derived by exactly removing the spurious $0\hbar\Omega$ center-of-mass (c.m.) motion.

This work is the first step in constructing a translationally invariant one-body density matrix in momentum space, although at present only a local one, from the given output of NCSM calculations. In Chapter 2, the concept of the many-body basis in the M-Scheme is introduced and an example with a toy Hamiltonian illustrates the action of a Hamiltonian on such a basis. In Chapter 3, the space-fixed local one-body density is constructed from the outputs of NCSM calculations. We concentrate on the nuclei $^4\text{He}$, $^6\text{He}$, and $^6\text{Li}$. In Chapter 4, we show how the spurious c.m. motion can be removed exactly to obtain translationally invariant local densities. With the latter we calculate root-mean-square radii as examples of observables. A summary and outlook is presented in Chapter 5. This thesis is supplemented with a set of Appendices that illustrate analytical derivations and numerical checks in detail.
2 MANY-BODY BASIS STATES

Performing the quantum mechanics for many-body systems, one commonly begins by representing the total wave function $|\Psi\rangle$ of the many-body system as a product of wave functions of the single particles in the system. This is especially useful when the single particle basis wave functions are orthonormal because the total wave function can be orthonormalized with little effort [17, 18]. Since this work concentrates on the nuclear many-body system involving neutrons and protons, which are fermions, the total wave function must be constructed through a Slater determinant as described in Section 2.1.

In addition, when dealing with non-relativistic quantum mechanics, the many-body system, and the states that create it, should obey Galilean invariance as well as other invariances like parity, charge, and particle number conservation. The above listed invariances are all Abelian symmetries which means that the quantum numbers for the many-body system are either the sum or the product of the quantum numbers from the single-particle states. Galilean invariance contains rotational as well as translational invariance. Assuming that the many-body Hamiltonian, $\hat{H}$, is rotationally invariant, requires that the operators of the total angular momentum, $\hat{J}^2$, and its projection on the z-axis, $\hat{J}_z$, commute with the Hamiltonian of the system, $\hat{H}$. This commutation requires that the eigenstates of $\hat{H}$ have the total angular momentum, $J$, and its third projection along the z-axis, $M$, as good quantum numbers. This fact will be explained when we describe a specific organization scheme, the M-scheme, for the many-body states in Section 2.2. A simple application of the M-scheme and a pairing Hamiltonian is discussed in Section 2.3.

2.1 Slater Determinants

A Slater determinant is an anti-symmetric linear combination of products of single particle states. Anti-symmetry is a requirement of all wave functions involving fermions.
As an example, a Slater determinant representing the total wave function $\Psi$ for 2 particles is given by

$$
\Psi(x_1, x_2) = \frac{1}{\sqrt{2!}} \begin{vmatrix}
\psi_1(x_1) & \psi_2(x_1) \\
\psi_1(x_2) & \psi_2(x_2)
\end{vmatrix} \equiv |\psi_1\psi_2|,
$$

(2.1)

where each particle coordinates are labeled as $x_i$ and each state is labeled by $\psi_i$.

To explain why a Slater determinant is necessary, suppose we start with a total wave function

$$
\Psi(x_i, x_j) = \psi_i(x_i) \psi_j(x_j),
$$

(2.2)

where the single particle states, $\psi_i$ and $\psi_j$, are orthonormal. If particle one’s coordinates, $x_i$, and two’s, $x_j$, are exchanged, then the new total wave function is not anti-symmetric since the resulting wave function has the same sign as the old wave function,

$$
\Psi(x_j, x_i) = \psi_i(x_j) \psi_j(x_i) = \Psi(x_i, x_j).
$$

(2.3)

The solution to this issue is a Slater determinant which provides a linear combination of products of single particle states as opposed to just a product,

$$
\Psi(x_i, x_j) = \frac{1}{\sqrt{2!}} \begin{vmatrix}
\psi_i(x_i) & \psi_j(x_i) \\
\psi_i(x_j) & \psi_j(x_j)
\end{vmatrix} = \frac{1}{\sqrt{2}} \left[ \psi_i(x_i) \psi_j(x_j) - \psi_j(x_i) \psi_i(x_j) \right].
$$

(2.4)

If we examine Eq. (2.4) we can easily see that for a swap of particle coordinates the wave function changes sign, thus fulfilling the condition of anti-symmetry,

$$
\Psi(x_j, x_i) = \frac{1}{\sqrt{2}} \left[ \psi_i(x_j) \psi_j(x_i) - \psi_j(x_j) \psi_i(x_i) \right] = -\Psi(x_i, x_j).
$$

(2.5)

The general form of a Slater determinant is

$$
\Psi(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix}
\psi_1(x_1) & \psi_2(x_1) & \ldots & \psi_N(x_1) \\
\psi_1(x_2) & \psi_2(x_2) & \ldots & \psi_N(x_2) \\
\vdots & \vdots & \ddots & \vdots \\
\psi_1(x_N) & \psi_2(x_N) & \ldots & \psi_N(x_N)
\end{vmatrix} \equiv |\psi_1 \ldots \psi_N|,
$$

(2.6)

where $N$ is the particle number of the system. The final notation in Eq. (2.6) is a compact notation for a Slater determinant.
2.2 The M-Scheme Basis

For a many-body Hamiltonian ($\hat{H}$) to be rotational invariant, $\hat{H}$ must fulfill the following commutation relations,

$$[\hat{H}, \hat{J}^2] = [\hat{H}, \hat{J}_z] = 0.$$  

(2.7)

This means that the eigenvalues of the total angular momentum, $J$, and the projection of $J$ on the z-axis, $M$, are good quantum numbers. In addition, $M$ is the sum of the eigenvalues $m_i$ in each single particle state [17–19],

$$M = \sum_{i=1}^{N} m_i,$$  

(2.8)

where $N$ is the number of single particle states representing the specific system under consideration. Thus, it is convenient to choose the many-body states that have the same $M$ as a basis for the total wave function. This combination of many-body states defines the M-scheme basis. When considering the operator $\hat{J}^2$, we are using its representation in terms of raising and lowering operators $\hat{J}^+$ and $\hat{J}^-$,

$$\hat{J}^2 = \frac{1}{2}(\hat{J}^- \hat{J}^+ + \hat{J}^+ \hat{J}^-) + \hat{J}_z^2$$

$$= \hat{J}^- \hat{J}^+ + \hat{J}_z(\hat{J}_z + 1).$$  

(2.9)

The operator $\hat{J}^+$ and $\hat{J}^-$ are the sum over the single particle $\hat{j}^+$ and $\hat{j}^-$ which obey

$$\hat{j}^\pm |\psi_{m_i}^j\rangle = \sqrt{j_i(j_i + 1) - m_i(m_i \pm 1)} |\psi_{m_i \pm 1}^j\rangle.$$  

(2.10)

We also know, that for each total $J$, there is a $(2J + 1)$ degeneracy for $M$. If we put $N_p$ protons and $N_n$ neutrons into a specific $J$ orbit, the number of possible configurations is $C_{N_p}^{2J+1} \times C_{N_n}^{2J+1}$, and the number of states in each nucleon’s basis increases in a combinatorial fashion. However, a computational advantage in this basis is that the occupied single particle state can be described bit wise, i.e. 1 as a state being occupied, 0 for not. This means, that despite the number of states increasing in such large numbers,
Figure 2.1: Comparison of the storage requirements in the J and the M-scheme. ‘Number of Matrix Elements’ on the right specifies how much memory is used to store each structure. ‘D’ in the right figure represents the dimension of the stored array. The equations above each line that include ‘D’ describe how the change in the dimension affects the matrix elements. [20]

the storage of the states in a numerical consideration can be performed very efficiently, as shown in Figure 2.1 [20].

One can also construct a J-scheme basis, where the basis states have a fixed $J$, and the many-body Hamiltonian is block diagonal in terms of $J$. In this case, each basis state must be represented as a linear combination of M-scheme states, according to standard angular momentum algebra. This requires more time to compute each element as well as the explicit storage of the states, which requires considerably more memory than the bit-wise storage of the M-scheme basis [17, 20]. Notice that in Fig. 2.1 the memory requirement of the J-scheme is considerably higher while having a lower dimension than the M-scheme.
In the following Section, an explicit example for constructing an M-scheme basis and applying it to a pairing Hamiltonian is given.

### 2.3 Application to a Pairing Hamiltonian

For a pairing Hamiltonian, creation and annihilation operators are used to manipulate the basis more easily as compared to conventional computational methods. A trade-off for simplifying the computation of applying the Hamiltonian to a system is that understanding such an abstract formalism is not trivial. Let us define a simple number operator

\[ \hat{G}^l_i = \hat{a}_i^\dagger \hat{a}_j, \]  

(2.11)

where \( \hat{a}_i^\dagger \) is a creation operator for the \( 'i' \) state and \( \hat{a}_j \) is an annihilation operator for the \( 'j' \) state. A creation operator \( \hat{a}_i^\dagger \) creates a particle in state \( 'i' \) as long as there is not a particle already in that state \( 'i' \). An annihilation operator \( \hat{a}_j \) destroys a particle in state \( 'j' \) as long as there is one to destroy. If either operator is applied on a state and the required conditions for the operator are not met, the wave function is zero.

For example, applying the number operator \( \hat{G}^l_i \) on a total wave function with three single particle states, \( |\Psi_{ijk}\rangle = |\psi_i\psi_j\psi_k\rangle \), results in

\[
\hat{G}^l_i |\Psi_{ijk}\rangle = \hat{a}_i^\dagger \hat{a}_j |\psi_i\psi_j\psi_k\rangle = \hat{a}_i^\dagger |\psi_j\psi_k\rangle = |\psi_l\psi_j\psi_k\rangle = |\Psi_{ljk}\rangle .
\]  

(2.12)

An example pairing Hamiltonian is used here to illustrate how this type of creation and annihilation operator formalism, along with M-Scheme, can result in the energy eigenvalues and eigenvectors of the system. First, let us introduce the Hamiltonian, \( \hat{H} \), as

\[
\hat{H} = -G \hat{P}_+ \hat{P}_-,
\]  

(2.13)
where $G$ is the strength of the pairing interaction (in this case a constant). The creation pairing operator $\hat{P}_+$ is defined as

$$\hat{P}_+ = \sum_i \hat{a}_{i,2m=1}^\dagger \hat{a}_{i,2m=-1}^\dagger .$$

(2.14)

and the annihilation pairing operator $\hat{P}_-$ is described by

$$\hat{P}_- = \sum_i \hat{a}_{i,2m=1} \hat{a}_{i,2m=-1} .$$

(2.15)

The variable ‘$i$’ in Eqs. (2.14) and (2.15) represents the $n$ quantum number of a single particle state (s.p.s.). The operator $\hat{P}_+$ in Eq. (2.14) creates pairs of single particle states. The operator $\hat{P}_-$ in Eq. (2.15) annihilates pairs of single particle states. By introducing a set of single particle states in Table 2.1, we can construct all the total wave functions with a desired M value and number of particles $A$ within this model space. Table 2.2 shows the total wave functions with the desired M value of ‘0’ and a particle number, $A = 2$. These

<table>
<thead>
<tr>
<th>index</th>
<th>$n$</th>
<th>$l$</th>
<th>$2j_i$</th>
<th>$2m_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>-1</td>
</tr>
</tbody>
</table>

combinations of single particle states represent the Slater determinant basis. To help understanding the interaction of the pairing Hamiltonian on these total wave functions, a matrix is created where each index of the matrix represents either an occupied many-body
state or an empty one. This matrix is given by

\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix},
\]

(2.16)

where the basis for the matrix is given by

\[
|\Psi_{1,2} \rangle, |\Psi_{1,4} \rangle, |\Psi_{2,3} \rangle, |\Psi_{3,4} \rangle
\]

Table 2.2: Single particle state combinations that have the total quantum number \(M = 0\). Each single particle state combination is represented by a Slater determinant. The total number of particles, \(A\), is 2.

<table>
<thead>
<tr>
<th>State Combinations with (M = \sum_i m_i = 0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(</td>
</tr>
<tr>
<td>(</td>
</tr>
<tr>
<td>(</td>
</tr>
<tr>
<td>(</td>
</tr>
</tbody>
</table>

Once a matrix is obtained in the desired M-Scheme basis, the pairing Hamiltonian is applied to each total wave function in the basis and the resulting total wave functions are stored. Table 2.3 gives the starting single particle state combinations as well as the resulting total wave functions that are occupied after application of \(\hat{H}\).
Table 2.3: Initial single particle state combinations used in the M-scheme basis as well as the resulting total wave functions that are occupied after application of the pairing Hamiltonian \( \hat{H} \). The factor of \( \frac{1}{\sqrt{2}} \) results from the normalization.

<table>
<thead>
<tr>
<th>Initial State</th>
<th>Final State Combination</th>
</tr>
</thead>
<tbody>
<tr>
<td>(</td>
<td>\Psi_{1,2}\rangle)</td>
</tr>
<tr>
<td>(</td>
<td>\Psi_{1,4}\rangle)</td>
</tr>
<tr>
<td>(</td>
<td>\Psi_{2,3}\rangle)</td>
</tr>
<tr>
<td>(</td>
<td>\Psi_{3,4}\rangle)</td>
</tr>
</tbody>
</table>

Once the pairing Hamiltonian has been applied, the results are stored in the M-scheme basis matrix,

\[
\begin{pmatrix}
1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1
\end{pmatrix}
\]

\(-\frac{G}{\sqrt{2}}\). \hspace{1cm} (2.17)

The matrix is then diagonalized to obtain the eigenvalues and eigenvectors in the M-scheme basis. The results of the diagonalization are shown in Table 2.4.

This is the general process of obtaining eigenvectors and eigenvalues using a M-scheme basis along with a pairing Hamiltonian. The formalism is summarized as follows. We begin with a set of single particle states. Then we take a desired \( M \) value and particle number \( A \) to construct a basis of all the Slater determinants with the fixed \( M \) value. After that, we apply a pairing Hamiltonian on the basis matrix. Lastly, we take the resulting matrix and find the eigenvalues and eigenvectors through diagonalization. This method, though simple in the previous case, can be expanded to more complex Hamiltonians, e.g. realistic two nucleon interactions, as well as applied to a much larger configuration space. In the following Chapters, we start with given eigenvectors from a M-scheme basis calculation of the NCSM and construct nuclear probability distributions.
Table 2.4: Eigenvalues and corresponding Eigenvectors from the diagonalization of the M-scheme basis matrix after application of the pairing Hamiltonian $\hat{H}$.

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>0.0</th>
<th>0.0</th>
<th>0.0</th>
<th>-2.0G</th>
</tr>
</thead>
<tbody>
<tr>
<td>Basis</td>
<td>Eigenvector</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$</td>
<td>\Psi_{1,2}\rangle$</td>
<td>$-\frac{1.0}{\sqrt{2.0}}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$</td>
<td>\Psi_{1,4}\rangle$</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$</td>
<td>\Psi_{2,3}\rangle$</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$</td>
<td>\Psi_{3,4}\rangle$</td>
<td>$\frac{1.0}{\sqrt{2.0}}$</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>
3 Space-Fixed Local One-Body Densities of the NCSM

Since its inception by Maria Goeppert-Mayer, in 1949 [21, 22], the nuclear single-particle shell model has been a successful approach to explain the structure of atomic nuclei. In its early realizations, it was necessary to use effective, phenomenological nucleon-nucleon (NN) interactions in a truncated model space to simulate various experimental phenomena. In the early stages of shell-model calculations only nucleons in the valence shell could be treated explicitly, while those in closed shells were approximated as an inert core.

With the advent of modern supercomputers the basis space in shell-model calculations could be dramatically increased, and for light nuclei the assumption of an inert core could be abandoned. In addition, it became possible to employ realistic NN interactions, i.e. those that describe two-nucleon observables with high precision, as well as three-nucleon interactions. This lead to the ab initio no-core shell model (NCSM), which first successfully described the energy spectrum of $^{12}$C [23, 24]. Up to now the NCSM is extremely successful in describing properties of ground and excited states of light nuclei, to about $A \approx 16$. For a review see Ref. [25].

NCSM calculations for $^4$He, $^6$He, and $^6$Li obtained from the Iowa State group (James Vary and Pieter Maris) use the J-Matrix Inverse Scattering Potential, fitted up to $A=16$, (JISP16) for the NN interaction [26]. In this work, matrix elements from the NCSM calculations are used to construct local one body densities in a space-fixed frame. In Section 3.1, some basic ideas of the NCSM are summarized. In Section 3.2, the foundation for obtaining the one-body local density is layed out. The following sections then show numerical results for $^4$He (Section 3.3), $^6$He (Section 3.4), and $^6$Li (Section 3.5).
3.1 Review of Basic Features of the NCSM

In this section, a brief summary of properties of the NCSM following Ref. [25] is given. The starting Hamiltonian of the \textit{ab initio} NCSM is given by

\[ H_A = \frac{1}{A} \sum_{i<j} \left( \mathbf{p}_i - \mathbf{p}_j \right)^2 \frac{1}{2m} + \sum_{i<j} V_{NN,i,j} + \sum_{i<j<k} V_{NNN,i,j,k} . \]  

(3.1)

Here \( m \) is the nucleon mass, which for our calculation is taken to be the average of neutron and proton masses, \( m = 938.920 \) MeV. The NN interaction is given by \( V_{NN,i,j} \), and the three-nucleon interaction by \( V_{NNN,i,j,k} \). The JISP16 NN interaction, employed in the calculations our study uses, is designed to mimic three-nucleon force contributions as they, e.g., occur for modern chiral NN forces, so that the last term can be omitted.

Though the Hamiltonian \( H_A \) of Eq. (3.1) is translationally as well as rotationally invariant, the Slater determinant basis used to diagonalize \( H_A \) is only rotationally invariant. The basis employed by the Iowa State group is an M-scheme basis.

To explicitly construct the Slater determinants, a harmonic oscillator (HO) basis is used since this basis allows preservation of translational symmetry of a bound nuclear system. The details on this will be given in Chapter 4.

A single nucleon HO wave function is given by

\[ \psi_{nlm}(\mathbf{r}, b) = R_{nl}(r, b) Y_{lm}(\hat{\mathbf{r}}) \]  

(3.2)

where \( R_{nl}(r, b) \) is the radial HO wave function. The HO length parameter \( b \) is related to the HO frequency \( \Omega \) as

\[ b = \sqrt{\frac{\hbar}{m\Omega}} . \]  

(3.3)

Here \( m \) is the average nucleon mass. The angular part is given by the standard spherical harmonics \( Y_{lm}(\hat{\mathbf{r}}) \equiv Y_{lm}(\theta, \phi) \). The radial wave function is explicitly given as

\[ R_{nl}(r, b) = \frac{\sqrt{2 \Gamma(n+1)}}{\sqrt{\Gamma\left(l + \frac{3}{2} + n\right)(b^2)^{l+\frac{1}{2}}}} r^l e^{-\frac{r^2}{2b^2}} L^l_{l+\frac{1}{2}}\left(\frac{r^2}{b^2}\right) , \]  

(3.4)
where $L_{n}^{l+rac{1}{2}}$ represents the associated Laguerre polynomials [27]. If a variable $\nu$ is defined as $\nu = \frac{mc^2\hbar}{2\hbar^2c^2} = \frac{1}{2\nu^2}$, then the radial wave function becomes,

$$R_{nl}(r, \nu) = \frac{\sqrt{2} (2\nu)^{l+rac{1}{2}} \Gamma(n+1)}{\sqrt{\Gamma(l + \frac{3}{2} + n)}} r^l e^{-\nu r^2} L_{n}^{l+rac{1}{2}}(2\nu r^2).$$  \hspace{1cm} (3.5)

The explicit derivation of $R_{nl}(r, \nu)$ is given in Appendix A. The single particle energies for the three-dimensional HO are given by [28]

$$\varepsilon_{nl} = \left(2n + l + \frac{3}{2}\right) \hbar \Omega. \hspace{1cm} (3.6)$$

The HO wave functions are complete and thus can be used as single-particle basis states for constructing the Slater determinants serving as the basis for the NCSM calculation. Since the model space for a computation must be finite, a truncation parameter $N_{\text{max}}$ is introduced, meaning that only many-body states with HO quanta up to $N_{\text{max}}$ are included in the basis. Physical observables should not depend on the basis in which the calculation is preformed. Thus in practice, $N_{\text{max}}$ is increased until the observable under consideration is converged with respect to $N_{\text{max}}$ [23–25].

After a calculation is completed, the energy eigenvalue of the Hamiltonian $H_A$ is obtained together with the wave function. In practice, the wave function is not stored after the computation, rather only the coefficients of the Slater determinants. Thus, to work with the many-body wave function it must be reconstructed using the coefficients as input.

### 3.2 The One-Body Density Matrix

Since wave functions are not quantum mechanical observables, one needs to define and compute observable quantities, e.g. a probability distribution. The one body-density matrix (OBDM) is one of the simplest many-body observables, describing the probability of finding particles at a specific position $r_A (r'_A)$. In its most general form it is given by [29]

$$\rho^{fi}(r'_A, r_A) = \int \Psi_i^*(r'_1, r_2, ..., r_A) \times \Psi_f(r_1, r_2, ..., r_A) d^3r_2...d^3r_A. \hspace{1cm} (3.7)$$
Here $\Psi_i$ represents the initial A-body wave function and $\Psi_f$ the final one. In the limit $\mathbf{r}_1 = \mathbf{r}_1'$ one obtains the local one-body density, and for $\Psi_i = \Psi_f$ this corresponds to the probability of finding a nucleon at position $\mathbf{r}_1$ when the system is in the state $\psi_{i=f}$,

$$\rho_{sf}^{\Omega}(\mathbf{r}_1) = \int \rho(\mathbf{r}_1, \mathbf{r}_1')\delta(\mathbf{r}_1 - \mathbf{r}_1')d^3r_1' \tag{3.8}$$

The index $\Omega$ indicates that the local one-body density in principle depends on the HO basis, and thus the HO energy scale, in which the $H_A$ of Eq. (3.1) has been computed. Due to the construction of that basis from single-particle states in single-particle coordinates, Eq. (3.8) is referred to as space-fixed (s.f.) density. This means that $\rho_{sf}^{\Omega}(\mathbf{r}_1)$ contains the motion of the center-of-mass (c.m.) and thus is not translationally invariant. How to remedy this situation will be laid out in Chapter 4. The one-body density distribution is a probability and is normalized to the number of nucleons

$$\int \rho_{sf}^{\Omega}(\mathbf{r}) \, d^3r = A. \tag{3.9}$$

Since we are using harmonic oscillator wave functions, and the space-fixed one-body density is a function of the vector $\mathbf{r}$, there is a dependence on the angles. We first perform a multipole expansion [29], to incorporate all contributions from different multipoles $K$,

$$\rho_{sf}(\mathbf{r}) = \sum_K^{2J} \frac{\langle JMK0|JM \rangle}{\sqrt{2J+1}} Y_K^0(\hat{r})\rho_{sf}^{(K)}(\mathbf{r}), \tag{3.10}$$

where $\rho_{sf}^{(K)}(\mathbf{r})$ is the $K$th multipole of the s.f. density.

This multipole expansion simplifies the Fourier transform to momentum space described in the following section as well as observable calculations in Chapter 4. With a HO single-particle basis, each multipole is given by

$$\rho_{sf}^{(K)}(\mathbf{r}) = \sum R_{n_{1l_1}}(r, \nu)R_{n_{2l_2}}(r, \nu) \frac{-1}{\sqrt{2K+1}} \left( \frac{1}{2} j_1 |Y_{K}| \frac{1}{2} j_2 \right) \times \langle A\lambda J||[\hat{a}_{n_{1l_1}}^\dagger \hat{a}_{n_{2l_2}}]^{(K)}||A\lambda J \rangle. \tag{3.11}$$

The $R_n(r)$’s are the radial components of the HO wave function described earlier in Eq. (3.5). The reduced matrix element of a spherical harmonic in Eq. (3.11) can be
represented by
\[ \left\langle l_1 \frac{1}{2} j_1 || Y_k || l_2 \frac{1}{2} j_2 \rightangle = \frac{1}{\sqrt{4\pi}} \hat{j}_1 \hat{j}_2 \hat{l}_2(-1)^{j_1+j_2} \langle l_1 0 l_2 0 | K 0 \rangle \times \begin{pmatrix} j_1 & j_2 & K \\ l_2 & l_1 & \frac{1}{2} \end{pmatrix} , \] (3.12)

using a Wigner-6J coefficient. (The Condon-Shortley convention is used for the Clebsch-Gordan coefficients [29].) The variable \( \hat{j} \) is defined as \( \hat{j} \equiv \sqrt{2j + 1} \).

Lastly, \( \langle A J || (a^+_n l_{1j_1} \tilde{a}_{n^* l_{2j_2}})^{(K)} || A J \rangle \) in Eq. (3.11) represents a reduced matrix element of the \( K \)th multipole of the OBDM [29]. This value is read in from files with the Maris-Vary input data [30]. A description of which values are read from the Maris-Vary files is contained in Appendix C. The explicit derivation of each multipole contribution \( (K = 0, 1, 2) \) to the total local density is given in Appendix B.

### 3.3 Fourier Transformation of the Position-Space to Momentum-Space Density

The momentum space distribution is obtained via a Fourier transform of \( \rho_{sf}(r) \),
\[ \rho_{sf}(q) = \int d^3r \rho_{sf}(r)e^{-iqr} , \] (3.13)
where \( q \) represents the momentum transfer. Inserting the multipole expansion of plane waves,
\[ e^{-iqr} = 4\pi \sum_{lm} Y^m_l(\hat{r})Y^m_l(\hat{q})(-i)^l j_l(qr) , \] (3.14)
leads to
\[ \rho_{sf}(q) = 4\pi \rho(r) \sum_{lm} Y^m_l(\hat{r})Y^m_l(\hat{q})(-i)^l j_l(qr)d^3r . \] (3.15)
Inserting Eq. (3.10) as the definition of \( \rho_{sf}(r) \) and defining the coefficient
\[ C_K = \frac{\langle JMK0|JM \rangle}{\sqrt{2J + 1}} , \] (3.16)
leads to
\[ \rho_{sf}(r) = \sum_K \frac{\langle JMK0|JM \rangle}{\sqrt{2J + 1}} Y^0_K(\hat{r}) \rho^{(K)}_{sf}(r) \]
\[ = \sum_K C_K Y^0_K(\hat{r}) \rho^{(K)}_{sf}(r) , \] (3.17)
and

\[
\rho_{sf}(\mathbf{q}) = 4\pi \int \sum_K C_K Y_K^0(\hat{r}) \rho_{sf}^{(K)}(r) \sum_{lm} Y_l^m(\hat{r}) Y_l^m(\hat{q})(-i)^j j_l(qr) d^3r
\]

\[
= 4\pi \sum_{lm} \sum_K C_K (-i)^l Y_l^m(\hat{q}) \int dr r^2 \rho_{sf}^{(K)}(r) j_l(qr) \int d\Omega Y_K^0(\hat{r}) Y_l^m(\hat{r}).
\] 

(3.18)

Noting that the integral over the angular part of the r-space is the completeness relation,

\[
\int d\Omega Y_K^0(\hat{r}) Y_l^m(\hat{r}) = \delta_{lk} \delta_{m0},
\]

(3.19)

we can carry out the triple sum and obtain the space-fixed momentum space diagonal density as

\[
\rho_{sf}(\mathbf{q}) = 4\pi \sum_K C_K (-i)^K Y_K^0(\hat{q}) \int dr r^2 \rho_{sf}^{(K)}(r) j_K(qr).
\]

(3.20)

Defining

\[
\tilde{\rho}_{sf}^{(K)}(q) = 4\pi \int dr r^2 \rho_{sf}^{(K)}(r) j_K(qr),
\]

(3.21)

Eq. (3.20) can be written as

\[
\rho_{sf}(\mathbf{q}) = \sum_K C_K (-i)^K Y_K^0(\hat{q}) \tilde{\rho}_{sf}^{(K)}(q).
\]

(3.22)

Equation (3.22) is the final representation of the Fourier transform of the space-fixed momentum space diagonal density. The momentum space density is normalized such that \(\rho_{sf}(q \to 0) = A\).

### 3.4 Space-Fixed Local Density for \(^4\text{He}\)

In this Section the normalization, the two-dimensional (2D) local density, and the three-dimensional (3D) local density are calculated and shown for the nucleus \(^4\text{He}\). The input information is obtained from Maris-Vary data sets, [30], with \(N_{\text{max}} = 2\) and 14, where \(N_{\text{max}} = 14\) represents a converged calculation with respect to the ground state binding energy. The major difference between \(N_{\text{max}} = 2\) and \(N_{\text{max}} = 14\) is the number of elements in the basis. For \(N_{\text{max}} = 2\) there are 36 basis states for both the protons and neutrons. To compare, the \(N_{\text{max}} = 14\) data files have 5007 basis states for both. In these two
calculations, the Coulomb interaction between the protons is neglected, so that the neutron and proton local densities are identical.

The normalization condition, Eq. (3.9), can be used to ensure our reconstruction of the space-fixed local density is correct. The data files contain separate coefficients for the proton and neutron density distributions, and thus they are separately reconstructed. Thus ‘A,’ the number of nucleons, in this Section’s results refer to either the number of neutrons or protons. The calculated normalization from the $N_{\text{max}} = 14$ data file is of the same accuracy as the one from the $N_{\text{max}} = 2$ data file and is therefore not shown.

For $^4\text{He}$, the normalization for the proton and neutron densities obtained from the $N_{\text{max}} = 2$ data file is 2 as shown in Table 3.1. The matter density has the expected normalization of 4 as shown in Table 3.1.

Table 3.1: The numerically obtained normalization, Eq. (3.9), for $^4\text{He}$ from the $N_{\text{max}} = 2$ data file. The order of the states, top to bottom, show the order of excitation energy levels. The calculations are based on a $N_{\text{max}} = 2$ NCSM calculation [30], which neglects the Coulomb interaction between the protons.

<table>
<thead>
<tr>
<th>State</th>
<th>Proton</th>
<th>Neutron</th>
<th>Matter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0^+_1$ g.s.</td>
<td>1.99999979</td>
<td>1.99999979</td>
<td>3.99999958</td>
</tr>
<tr>
<td>$0^+_2$</td>
<td>1.99999980</td>
<td>1.99999980</td>
<td>3.99999961</td>
</tr>
<tr>
<td>2$^-$</td>
<td>1.99999989</td>
<td>1.99999989</td>
<td>3.99999977</td>
</tr>
<tr>
<td>4$^+$</td>
<td>1.99999978</td>
<td>1.99999978</td>
<td>3.99999956</td>
</tr>
<tr>
<td>1$^-$</td>
<td>1.99999993</td>
<td>1.99999993</td>
<td>3.99999985</td>
</tr>
</tbody>
</table>

To more accurately compare the convergence of the $N_{\text{max}} = 2$ and $N_{\text{max}} = 14$ data sets, Table 3.2 shows the ground state binding energy for $^4\text{He}$ from the NCSM calculations compared to the experimental value. The experimental value cited is given with smaller
error then the accuracy shown. The $N_{\text{max}} = 2$ data set underbinds the ground state by almost 4 MeV. The $N_{\text{max}} = 14$ data set provides a binding energy for the ground state that compares more favorably with experiment though it still overestimates it by about 900 keV. Comparing $N_{\text{max}} = 14$ and $N_{\text{max}} = 16$ binding energies, we can see that $N_{\text{max}} = 14$ is converged with respect to the ground state binding energy.

Table 3.2: The ground state binding energies (in MeV) for $^4$He from the $N_{\text{max}} = 2$, 14, and 16 data files as well as the experimental value. The results are based on a NCSM calculation [30], which neglects the Coulomb interaction between the protons. The experimental value is taken from Ref. [31, 32].

<table>
<thead>
<tr>
<th>State</th>
<th>$N_{\text{max}} = 2$</th>
<th>$N_{\text{max}} = 14$</th>
<th>$N_{\text{max}} = 16$</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0^+_1$ g.s.</td>
<td>24.478</td>
<td>29.160</td>
<td>29.163</td>
<td>28.29566</td>
</tr>
</tbody>
</table>

In Fig. 3.1, the space-fixed (s.f.) local density is shown for the ground state of $^4$He, computed from the $N_{\text{max}} = 2$ and $N_{\text{max}} = 14$ data files, as a function of the distance $r$ from the origin and the momentum transfer $q$. In panel (b), the momentum space local density distributions are multiplied by $Y_0^0(\theta, \phi)$ to ensure the normalization $\rho^{(0)}(q = 0) = A$. The position space portion in Fig. 3.1 shows that raising $N_{\text{max}}$ increases the local density close to the origin, i.e. before about 1 fm, but the rest of the density stays the same.

This comparison between $N_{\text{max}} = 2$ and $N_{\text{max}} = 14$ is displayed more clearly in Fig. 3.2 which depicts the absolute difference between the local densities for $^4$He in the ground state. In Fig. 3.2, the momentum space absolute difference in panel (b) shows a smaller maximum difference than the position space in panel (a). In addition, the difference in the coordinate space plot decreases to zero as $r$ increases while the momentum space difference increases out to about 2 fm$^{-1}$ and then decreases to zero.
Figure 3.1: The diagonal space-fixed local density $\rho^{(0)}(r)$ and $\rho^{(0)}(q)$ of the ground state, $0^+$, protons for $^4$He ($N_{\text{max}} = 2$ and $N_{\text{max}} = 14$). Panel (a) shows the coordinate space density, while panel (b) depicts the momentum space density, with $\rho^{(0)}(q)$ multiplied by $Y_0(\hat{q})$. 
Figure 3.2: The absolute difference of the s.f. local densities $\rho_{sf}^{(0)}(r)$ (panel (a)) and $\rho_{sf}^{(0)}(q)$ (panel (b)) between the calculations with $N_{\text{max}} = 2$ and $N_{\text{max}} = 14$ for the ground state, $0^+$, of $^4\text{He}$.

The s.f. local densities of the $1^-$ excited state for $^4\text{He}$ are shown in Fig. 3.3 for both $N_{\text{max}} = 2$ and $N_{\text{max}} = 14$ data sets as a function of $r$ as well as $q$. In panels (b) and (d), the $K=0$ part of the momentum space local density is multiplied by $Y_0^0(\theta, \phi)$ to ensure the normalization $\rho^{(0)}(q = 0) = A$. The $K=2$ pieces of the excited state in Fig. 3.3 are multiplied by a factor of 20 to increase the visibility of the features. The change of an
increase in $N_{\text{max}}$ on the local density in Fig. 3.3 decreases the maximum of the position space density by a factor of about three and falls off more slowly. This is clear when examining Fig. 3.3 around 3 fm, in panels (a) and (c), the probability is still visibly non-zero in the $N_{\text{max}} = 14$ data set but not in the $N_{\text{max}} = 2$ version. An important note with respect to the momentum space part of Fig. 3.3, panels (b) and (d), is that the $K = 2$ contribution is clearly diminished for $N_{\text{max}} = 14$ as compared to $N_{\text{max}} = 2$. 
Figure 3.3: The diagonal space-fixed local density $\rho^{(K)}(r)C_K$ and $\rho^{(K)}(q)C_K$ of the $1^-$ excited state of $^4\text{He}$ ($N_{\text{max}} = 2$ and $N_{\text{max}} = 14$). Panel (a) gives the coordinate space density for $N_{\text{max}} = 2$, with $\rho^{(2)}(r)$ multiplied by a factor of 20. Panel (b) depicts the momentum space density for $N_{\text{max}} = 2$, with $\rho^{(0)}(q)$ multiplied by the $Y_0^0(\hat{q})$ and $\rho^{(2)}(q)$ is multiplied by a factor of 20. Panel (c) gives the coordinate space density for $N_{\text{max}} = 14$, with $\rho^{(2)}(r)$ multiplied by a factor of 20. Panel (d) depicts the momentum space density for $N_{\text{max}} = 14$, with $\rho^{(0)}(q)$ multiplied by the $Y_0^0(\hat{q})$ and $\rho^{(2)}(q)$ is multiplied by a factor of 20.
The local density of Eq. (3.10) is a function of the vector variable $\mathbf{r}$,
\[ \rho_{sf}(\mathbf{r}) \equiv \rho_{sf}(r, \theta, \phi), \]
where the angular behavior is dictated by the spherical harmonics $Y_{l}^{m}(\theta, \phi)$. Therefore, the local density is rotationally symmetric about the $z$-axis when $m = 0$. Our calculations in this Section use $M = 0$ when describing the quantum state and thus the $\phi$ component of the local density is trivial and does not need to be shown. The full description of the local density can be captured when $N_{\text{max}} = 2$ or 14 are employed through the radial component $r$ and the azimuthal angle $\theta$.

In Fig. 3.1, the magnitude of the local density for $^4$He in the ground state is different, when $N_{\text{max}}$ is increased, near the origin while exhibiting the same fall-off when moving to larger $r$. Thus, it is not relevant to show both $N_{\text{max}}$ data sets in the 3D plot of the ground state of $^4$He. We give the space-fixed local density for the $N_{\text{max}} = 14$ data set in Fig. 3.4 because it is a converged calculation. The ground state of $^4$He in Fig. 3.4 is clearly spherical since there is no change in the density along the $\theta$-axis.
Figure 3.4: The proton diagonal s.f. local density $\rho(r)$ and $\rho(q)$ shown as a function of the radial coordinates $r$ (panel (a)), momentum transfer $q$ (panel (b)), and the azimuthal angle $\theta$ for the ground state, $0^+$, of $^4$He ($N_{\text{max}} = 14$).

For the excited state $1^-$ of $^4$He, we show in Fig. 3.5 and 3.6 both $N_{\text{max}} = 2$ and 14 data sets in order to provide a clear contrast between the size of the probability distributions.

The position space local density $\rho_{s,f}(r)$ is shown in Fig. 3.5 with $N_{\text{max}} = 2$ in panel (a) and $N_{\text{max}} = 14$ in panel (b). It should be noted that even the excited state $1^-$ of $^4$He, with higher order multipole components, is spherical as shown in Fig. 3.5. In Fig. 3.5 the width
of the half-maximum is around 2 fm in panel (b) and only around 1.2 fm in panel (a). This means that the increase of $N_{\text{max}}$ from 2 to 14 extends the distribution along $r$. Another note of difference between panels (a) and (b) in Fig. 3.5 is that the maximum probability density reached by $N_{\text{max}} = 14$ is a little less than half of what $N_{\text{max}} = 2$ reaches at $r = 0$, as indicated in the color scale.

The momentum space local density $\rho_{sf}(q)$ is given in Fig. 3.6 with $N_{\text{max}} = 2$ in panel (a) and $N_{\text{max}} = 14$ in panel (b). In this figure the 3D momentum space local density shows $N_{\text{max}} = 14$ more compact along $q$ than $N_{\text{max}} = 2$. This is the expected result from a Fourier transfer of such a distribution in position space. The momentum space 3D figure shows the excited state of $^4\text{He}$ as spherical, as it should since the Fourier transform should not affect the $\theta$ dependence of the density.
Figure 3.5: Panel (a): The proton diagonal s.f. local density $\rho(r)$ shown as a function of the radial coordinates $r$ and the azimuthal angle $\theta$ for the excited state, $1^-$, of $^4$He ($N_{\text{max}} = 2$).

Panel (b): The proton diagonal s.f. local density $\rho(r)$ shown as a function of the radial coordinates $r$ and the azimuthal angle $\theta$ for the excited state, $1^-$, of $^4$He ($N_{\text{max}} = 14$).
Figure 3.6: Panel (a): The proton diagonal s.f. local density $\rho(q)$ shown as a function of the momentum transfer $q$ and the azimuthal angle $\theta$ for the excited state, $1^-$, of $^4\text{He}$ ($N_{\text{max}} = 2$). Panel (b): The proton diagonal s.f. local density $\rho(q)$ shown as a function of the momentum transfer $q$ and the azimuthal angle $\theta$ for the excited state, $1^-$, of $^4\text{He}$ ($N_{\text{max}} = 14$).
3.5 Space-Fixed Local Density for $^6\text{He}$

In this Section, the normalization, two-dimensional (2D) local density, and the three-dimensional (3D) local density are calculated and shown for the nucleus $^6\text{He}$. The input information (reduced matrix elements of the interaction) for these calculations is obtained from Maris-Vary data files with $N_{\text{max}} = 2$ and 14 [30]. The $N_{\text{max}} = 2$ data set has 184 basis states for protons and neutrons combined. The $N_{\text{max}} = 14$ data set has 12160 basis states for protons and neutrons combined. The $N_{\text{max}} = 14$ data set is not converged, with respect to the ground state binding energy. This non-convergence is due mainly to the expansion of the local density from the addition of 2 neutrons, with respect to $^4\text{He}$. In addition, the harmonic oscillator basis does not converge easily due to the tail of the actual density falling off like $e^{-\alpha' r}$ while the HO basis has a $e^{-\alpha r^2}$ slope, where $\alpha$ and $\alpha'$ are arbitrary constants, at high $r$ values. In this calculation of $^6\text{He}$, the Coulomb interaction between the protons is neglected.

For $^6\text{He}$, the normalization of the densities obtained from the $N_{\text{max}} = 2$ data set are of the same accuracy as the $N_{\text{max}} = 14$ data set and are therefore not shown. The normalization for the proton densities in $^6\text{He}$ is 2 as shown in Table 3.3. The neutron density has a normalization of 4 and the matter density has one of 6, also shown in Table 3.3.

To more accurately compare the convergence of the $N_{\text{max}} = 2$ and $N_{\text{max}} = 14$ data sets, Table 3.4 shows the ground state binding energy for $^6\text{He}$ from the NCSM calculations with the experimental value. The $N_{\text{max}} = 2$ data set underbinds the ground state by over 12 MeV. The $N_{\text{max}} = 14$ data set provides a binding energy for the ground state that is almost exactly equal to experiment. From comparing the $N_{\text{max}} = 14$ and $N_{\text{max}} = 16$ we can consider $N_{\text{max}} = 14$ converged with respect to the binding energy of the ground state.
Table 3.3: The numerically obtained normalization for $^6$He from the $N_{\text{max}} = 2$ data file. The order of the states, top to bottom, show the order of excitation energy levels. The calculations are based on a $N_{\text{max}} = 2$ NCSM calculation [30], which neglects the Coulomb interaction between the protons.

<table>
<thead>
<tr>
<th>State</th>
<th>Proton</th>
<th>Neutron</th>
<th>Matter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0^+_1 \text{ g.s.}$</td>
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<td>5.99999989</td>
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<tr>
<td>$2^+_1$</td>
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<td>4.00000000</td>
<td>5.99999998</td>
</tr>
<tr>
<td>$2^+_2$</td>
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<td>5.99999994</td>
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<tr>
<td>$1^-_0$</td>
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<tr>
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<td>1.99999994</td>
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<td>5.99999982</td>
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</table>

Table 3.4: The ground state binding energies (in MeV) for $^6$He from the $N_{\text{max}} = 2$, 14, and 16 data files as well as the experimental value. The results are based on a NCSM calculation [30], which neglects the Coulomb interaction between the protons. The experimental value is taken from Ref. [31, 32].

<table>
<thead>
<tr>
<th>State</th>
<th>$N_{\text{max}} = 2$</th>
<th>$N_{\text{max}} = 14$</th>
<th>$N_{\text{max}} = 16$</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0^+_1 \text{ g.s.}$</td>
<td>17.108</td>
<td>29.270</td>
<td>29.397</td>
<td>29.271114 ± 0.000054</td>
</tr>
</tbody>
</table>

The proton space-fixed local density for the ground state of $^6$He computed from the $N_{\text{max}} = 2$ and 14 data sets is shown in Fig. 3.7. Panel (a) in the figure shows the local density as a function of the distance $r$ from the origin while panel (b) shows it as a function of the momentum transfer $q$. In panel (b), the momentum space local density plot, the distributions are multiplied by $Y^{(0)}_0(\theta, \phi)$ to ensure normalization, $\rho^{(0)}(q = 0) = A$. The position space density plot in Fig. 3.7 shows that as $N_{\text{max}}$ increases, the maximum probability density decreases at the origin. This is in contrast to $^4$He where the opposite happens. The position space portion in Fig. 3.7 shows that increasing the $N_{\text{max}}$ decreases
the local density close to the origin, i.e. before about 2 fm, but the probability is shifted to larger \( r \) values.

![Graph](image)

**Figure 3.7:** The proton diagonal space-fixed local density \( \rho^0(r) \) and \( \rho^0(q) \) of the ground state, \( 0^+ \), for \( ^6\text{He} \) (\( N_{\text{max}} = 2 \) and \( N_{\text{max}} = 14 \)). Panel (a) shows the coordinate space density, while panel (b) depicts the momentum space density, with \( \rho^0(q) \) multiplied by \( Y^0_0(\hat{q}) \).

A comparison between the proton local densities of \( ^4\text{He} \) and \( ^6\text{He} \) for \( N_{\text{max}} = 14 \) is given in Fig. 3.8. This figure shows a clear difference in scale of the two densities but only a slight difference in distribution since both fall off at about the same \( r \) value of 3 fm. It is interesting that the density for \( ^6\text{He} \) is much lower near the origin but still has a normalization of 2 because of the slightly higher density around 1.7 fm and beyond.
Figure 3.8: The proton diagonal space-fixed local density $\rho^{(0)}(r)$ and $\rho^{(0)}(q)$ of the ground state, $0^+$, for $^6$He and $^4$He ($N_{\text{max}} = 14$). Panel (a) shows the coordinate space density, while panel (b) depicts the momentum space density, with $\rho^{(0)}(q)$ multiplied by $Y_0^0(\hat{q})$. 
Figure 3.9: The neutron diagonal space-fixed local density $\rho^{(0)}(r)$ and $\rho^{(0)}(q)$ of the ground state, $0^+$, for $^6$He ($N_{max} = 2$ and $N_{max} = 14$). Panel (a) shows the coordinate space density, while panel (b) depicts the momentum space density, with $\rho^{(0)}(q)$ multiplied by $Y_0^0(\hat{q})$.

The neutron space-fixed local density for the ground state of $^6$He computed from the $N_{max} = 2$ and 14 data sets is shown in Fig. 3.9. In panel (b), the momentum space local density plot, the distributions are multiplied by $Y_0^0(\theta, \phi)$ to ensure the normalization, $\rho^{(0)}(q = 0) = A$. The position space density shown in Fig. 3.9 indicates that as $N_{max}$ increases, the maximum probability density decreases at the origin, same as in Fig. 3.7 for the proton density. The neutron density falls off much slower as a function of $r$ than the proton one, as shown by the value of $\rho^{(0)}(r)$ at 3 fm in panel (a). This slower decrease of the density is readily understood when one has in mind that $^6$He is considered a halo nucleus. Increasing $N_{max}$ pushes probability to larger $r$, though it still falls off as $e^{-\alpha' r^2}$ and not like $e^{-\alpha r}$ as a halo picture suggests [5].

The diagonal space-fixed local density of the $2^+$ excited state for $^6$He is shown in Fig. 3.10 for both $N_{max} = 2$ and 14. The proton density of the excited state is given in panels (a) and (b) while the neutron density is given in panels (c) and (d). The $K=2$ components of the proton local density in panels (a) and (b) are multiplied by a factor of
20 to make details more apparent. The K=2 components of the neutron local density in panels (c) and (d) are multiplied by only a factor of 5 for visibility. In panels (b) and (d), the momentum space local density plots, the K= 0 part of the distribution is multiplied by $Y_0^0(\theta, \phi)$ to ensure the normalization. The proton and neutron distributions of $^6$He for the excited state $2^+$ in Fig. 3.10 show two main differences between $N_{\text{max}} = 2$ and 14. First, the maximum of the position space local density is smaller at the origin. Secondly, the higher order multipole contribution is greater in the $N_{\text{max}} = 14$ data set than $N_{\text{max}} = 2$. However, the neutron local density in panel (c) shows a lower contribution by $\rho_{sf}^{(2)}$ when increasing $N_{\text{max}}$. 
Figure 3.10: The diagonal space-fixed local density $\rho^{(K)}(r)C_K$ and $\rho^{(K)}(q)C_K$ of the first $2^+$ excited state of $^6$He ($N_{max} = 2$ and $N_{max} = 14$). Panel (a) gives the proton coordinate space density, with $\rho^{(2)}(r)$ multiplied by a factor of 20. Panel (b) depicts the proton momentum space density, with $\rho^{(0)}(q)$ multiplied by the $Y_0^0(\hat{q})$ and $\rho^{(2)}(q)$ is multiplied by a factor of 20. Panel (c) gives the neutron coordinate space density, with $\rho^{(2)}(r)$ multiplied by a factor of 5. Panel (d) depicts the neutron momentum space density, with $\rho^{(0)}(q)$ multiplied by the $Y_0^0(\hat{q})$ and $\rho^{(2)}(q)$ is multiplied by a factor of 5.
As described in Section 3.5, the $\phi$ component of the local density is trivial and does not need to be shown. The proton density in Fig. 3.7 is very similar to the proton density for $^4$He and thus not of interest. The 3D neutron density of $^6$He with $N_{\text{max}} = 14$ is shown in Fig. 3.11 for position and momentum space. The $N_{\text{max}} = 2$ data set is not shown because the difference between the two is the magnitudes and not the distribution. As expected, the ground state of $^6$He is spherical, similar to $^4$He, though the local density of $^6$He falls off more slowly than the two neutron profile in $^4$He as discussed in Fig 2.9.

![Diagram](image)

Figure 3.11: The neutron diagonal space-fixed local density $\rho(r)$ and $\rho(q)$ shown as a function of the radial coordinates $r$ (panel (a)), momentum transfer $q$ (panel (b)), and the azimuthal angle $\theta$ for the ground state, $0^+$, of $^6$He ($N_{\text{max}} = 14$).
In the excited state $2^+$ of $^6$He the first non-spherical behavior is seen. In Fig. 3.12 the proton s.f. local density of the $2^+$ state in position space is shown for both, $N_{\text{max}} = 2$ and $14$, as a function of $r$ and $\theta$. It is immediately apparent that the difference for the proton density is small as $N_{\text{max}}$ increases. This is shown through the maximum density being almost equal, $0.13 \approx 0.11$, and the half-maximum being in roughly the same position, 1.3 fm. It is interesting to note that the proton density is still spherical even in an excited state.

Figure 3.12: Panel (a): The proton diagonal space-fixed local density $\rho(r)$ shown as a function of the radial coordinates $r$ and the azimuthal angle $\theta$ for the excited state, $2^+$, of $^6$He ($N_{\text{max}} = 2$). Panel (b): The diagonal space-fixed local density $\rho(r)$ shown as a function of the radial coordinates $r$ and the azimuthal angle $\theta$ for the 2nd excited state, $2^+$, of $^6$He ($N_{\text{max}} = 14$).
The neutron s.f. local density of the $2^+$ state is shown in Fig. 3.13 for $N_{\text{max}} = 2$ and 14 as a function of $r$ and $\theta$. The first detail to note is that the distribution is oblate with a slight bulge towards the center, 90 deg, and a depression at the top, 0 deg, and bottom, 180 deg. The bulge is not as apparent in the $N_{\text{max}} = 14$ data set which is consistent with the decrease in the multipole contribution in Fig. 3.10.

![Figure 3.13](image)

**Figure 3.13**: Panel (a): The neutron diagonal space-fixed local density $\rho(\mathbf{r})$ shown as a function of the radial coordinates $r$ and the azimuthal angle $\theta$ for the excited state, $2^+$, of $^6\text{He}$ ($N_{\text{max}} = 2$). Panel (b): The diagonal space-fixed local density $\rho(\mathbf{r})$ shown as a function of the radial coordinates $r$ and the azimuthal angle $\theta$ for the 2nd excited state, $2^+$, of $^6\text{He}$ ($N_{\text{max}} = 14$).
The neutron s.f. local density of the $2^+$ state in momentum space for $N_{\text{max}} = 2$ and 14 is shown in Fig. 3.14 as a function of $q$ and $\theta$. The oblate distribution of the position space for the neutron density is reversed in the momentum space plot of Fig. 3.14. This is to be expected because a Fourier transform does not act on the azimuthal angle $\theta$.

Figure 3.14: Panel (a): The neutron diagonal space-fixed local density $\rho(\mathbf{q})$ shown as a function of the momentum transfer $q$ and the azimuthal angle $\theta$ for the excited state, $2^+$, of $^6\text{He}$ ($N_{\text{max}} = 2$). Panel (b): The diagonal space-fixed local density $\rho(\mathbf{q})$ shown as a function of the momentum transfer $q$ and the azimuthal angle $\theta$ for the 2nd excited state, $2^+$, of $^6\text{He}$ ($N_{\text{max}} = 14$).
3.6 Space-Fixed Local Density for $^6$Li

In this Section, the normalization, two-dimensional (2D) local density, and the three-dimensional (3D) local density is calculated and shown for the nucleus $^6$Li. The $^6$Li nucleus has 3 protons and 3 neutrons which can naively be considered as 2 protons and 2 neutrons in the s-shell while the third proton and neutron are in the p-shell. This is a very similar picture to the $^6$He cluster model and thus we might expect analogies between the two nuclei.

The Maris-Vary data files used for this calculation are $N_{\text{max}} = 2$ and 14 [30]. The $N_{\text{max}} = 2$ data set has 184 basis states for protons and neutrons combined. The $N_{\text{max}} = 14$ data set has 12160 basis states for protons and neutrons combined. The $N_{\text{max}} = 14$ data set is not converged, similar to $^6$He, with respect to the ground state binding energy. This non-convergence is due to the extension of the local density with respect to the distance from the c.m. In this calculation of $^6$Li, the Coulomb interaction between the protons is neglected and thus the proton and neutron local densities are identical, therefore only the proton distributions are shown.

For $^6$Li, the normalization of the densities obtained from the $N_{\text{max}} = 2$ data set are of the same accuracy as the $N_{\text{max}} = 14$ data set and are therefore not shown. The normalization for the proton and neutron densities in $^6$He is 3 as shown in Table 3.5. The matter density normalization is 6, also shown in Table 3.5.

To more accurately compare the convergence of the $N_{\text{max}} = 2$ and $N_{\text{max}} = 14$ data sets, Table 3.6 shows the ground state binding energy for $^6$Li from the NCSM calculations with the experimental value. The $N_{\text{max}} = 2$ data set underbinds the ground state by over 12 MeV. The $N_{\text{max}} = 14$ data set provides a binding energy for the ground state that compares much more favourably with experiment though it still overestimates it by about 1.5 MeV. We can see from the comparison of $N_{\text{max}} = 14$ and $N_{\text{max}} = 16$ that the binding energy is almost converged for $N_{\text{max}} = 14$. 
Table 3.5: The numerically obtained normalization for $^6$Li from the $N_{\text{max}} = 2$ data file. The order of the states, top to bottom, show the order of excitation energy levels. The calculations are based on a $N_{\text{max}} = 2$ NCSM calculation [30], which neglects the Coulomb interaction between the protons.

<table>
<thead>
<tr>
<th>State</th>
<th>Proton</th>
<th>Neutron</th>
<th>Matter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1^+_1$ g.s.</td>
<td>3.00000019</td>
<td>3.00000019</td>
<td>6.00000039</td>
</tr>
<tr>
<td>$3^+$</td>
<td>3.00000008</td>
<td>3.00000008</td>
<td>6.00000017</td>
</tr>
<tr>
<td>$0^+$</td>
<td>2.99999973</td>
<td>2.99999973</td>
<td>5.99999945</td>
</tr>
<tr>
<td>$2^+$</td>
<td>2.99999967</td>
<td>2.99999967</td>
<td>5.99999934</td>
</tr>
<tr>
<td>$1^+_2$</td>
<td>2.99999990</td>
<td>2.99999990</td>
<td>5.99999980</td>
</tr>
</tbody>
</table>

Table 3.6: The ground state binding energies (in MeV) for $^6$Li from the $N_{\text{max}} = 2$, 14, and 16 data files as well as the experimental value. The results are based on a NCSM calculation [30], which neglects the Coulomb interaction between the protons. The experimental value is taken from Ref. [31, 32].

<table>
<thead>
<tr>
<th>State</th>
<th>$N_{\text{max}} = 2$</th>
<th>$N_{\text{max}} = 14$</th>
<th>$N_{\text{max}} = 16$</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1^+_1$ g.s.</td>
<td>19.292</td>
<td>33.001</td>
<td>33.119</td>
<td>31.993986 ± 0.0000001</td>
</tr>
</tbody>
</table>

The proton space-fixed local density for the ground state $1^+$ of $^6$Li, computed from the $N_{\text{max}} = 2$ and 14 data sets, is shown in Fig. 3.15. Panel (a) in the figure shows the local density as a function of the distance $r$ from the origin while panel (b) shows it as a function of the momentum transfer $q$. In panel (b), the momentum space local density plot, the distributions are multiplied by $Y_0^0(\theta, \phi)$ to ensure the normalization, $\rho(0)(q = 0) = A$. The K=2 components of the proton local density in panels (a) and (b) are multiplied by a factor of 5 to make details more apparent. The position space density plot, panel (a), in Fig. 3.15 shows that as $N_{\text{max}}$ increases, the maximum probability density of
\(\rho_{sf}^{(0)}(r)\) decreases at the origin. This is similar to the 1\(^-\) excited state of \(^4\)He and the 2\(^+\) excited state of \(^6\)He. The K= 2 contribution decreases as \(N_{\text{max}}\) increases following a similar pattern as the 1\(^-\) excited state of \(^4\)He.

![Graphs showing the behavior of local density\(\rho^K(r)\) and \(\rho^K(q)\) for \(^6\)Li.](image)

Figure 3.15: The diagonal space-fixed local density \(\rho^{(K)}(r)C_K\) and \(\rho^{(K)}(q)C_K\) of the ground state, 1\(^+\), for \(^6\)Li (\(N_{\text{max}}=2\) and \(N_{\text{max}}=14\)). Panel (a) shows the coordinate space density, while panel (b) depicts the momentum space density, with \(\rho^{(0)}(q)\) multiplied by \(Y_0^0(\hat{q})\).

The proton space-fixed local density for the excited state 3\(^+\) of \(^6\)Li, computed from the \(N_{\text{max}} = 2\) and 14 data sets, is shown in Fig. 3.16. Panel (a) in the figure shows the local density as a function of \(r\) while panel (b) shows it as a function of \(q\). In panel (b), the momentum space local density plot, the distributions are multiplied by \(Y_0^0(\theta, \phi)\) to ensure the normalization. The K=2 components of the proton local density in panels (a) and (b) are multiplied by a factor of 5 to make details more apparent. The position space density plot, panel (a), in Fig. 3.16 shows that as \(N_{\text{max}}\) increases, the maximum probability density of \(\rho_{sf}^{(0)}(r)\) decreases at the origin, same as the ground state. The K= 2 contribution decreases as \(N_{\text{max}}\) increases, similar to the ground state.
Figure 3.16: The proton diagonal s.f. local density $\rho^{(K)}(r)C_K$ and $\rho^{(K)}(q)C_K$ of the $3^+$ excited state of $^6$Li ($N_{max} = 2$ and $N_{max} = 14$). Panel (a) gives the coordinate space density for $N_{max} = 2$, with $\rho^{(2)}(r)$ multiplied by a factor of 5. Panel (b) depicts the momentum space density for $N_{max} = 2$, with $\rho^{(0)}(q)$ multiplied by the $Y^0_0(\hat{q})$ and $\rho^{(2)}(q)$ is multiplied by a factor of 5.

As described in Section 3.5, the $\phi$ component of the local density is trivial and does not need to be shown. The 3D proton density of the ground state $1^+$ for $^6$Li with $N_{max} = 2$ and 14 is shown in Fig. 3.17 for position space. The ground state of $^6$Li is not spherical like $^4$He and $^6$He. Instead, the density has a slight bulge at 90 deg. The proton local density of $^6$Li is slightly extended at the far $r$ values (past 3 fm). This seems reasonable when one considers that a simple shell model picture would have two protons in the s-shell and one proton in the p-shell. The 3D proton density of the ground state $1^+$ for $^6$Li in momentum space is shown in Fig. 3.18. The non-spherical nature of the ground state $1^+$ is even more difficult to see in Fig. 3.18. The change due to $N_{max}$ increasing in both Fig. 3.17 and 3.18 is not very noticeable for the 3D plot of the $1^+$ state.
Figure 3.17: Panel (a): The proton diagonal s.f. local density $\rho(r)$ shown as a function of the radial coordinates $r$ and the azimuthal angle $\theta$ for the ground state, $1^+$, of $^6$Li ($N_{\text{max}} = 2$).

Panel (b): The proton diagonal s.f. local density $\rho(r)$ shown as a function of the radial coordinates $r$ and the azimuthal angle $\theta$ for the ground state, $1^+$, of $^6$Li ($N_{\text{max}} = 14$).
The 3D proton density of the excited state $3^+$ for $^6\text{Li}$ with $N_{\text{max}} = 2$ and 14 is shown in Fig. 3.19 for position space. The position space density of the excited state $3^+$ is prolate with bulges at the top, 0 deg, and bottom, 180 deg. The 3D proton density of the excited
state $3^+$ for $^6$Li in momentum space is shown in 3.20. The distribution of the excited state in momentum space again is inverted, just like the $2^+$ state of $^6$He. The change due to $N_{\text{max}}$ increasing in both Fig. 3.19 and 3.20 is not very noticeable for the 3D plot of the $3^+$ state.

![Figures 3.19](image)

Figure 3.19: Panel (a): The proton diagonal s.f. local density $\rho(r)$ shown as a function of the radial coordinates $r$ and the azimuthal angle $\theta$ for the excited state, $3^+$, of $^6$Li ($N_{\text{max}} = 2$). Panel (b): The proton diagonal s.f. local density $\rho(r)$ shown as a function of the radial coordinates $r$ and the azimuthal angle $\theta$ for the excited state, $3^+$, of $^6$Li ($N_{\text{max}} = 14$).
Figure 3.20: Panel (a): The proton diagonal s.f. local density $\rho(q)$ shown as a function of the momentum transfer $q$ and the azimuthal angle $\theta$ for the excited state, $3^+$, of $^6\text{Li}$ ($N_{\text{max}} = 2$). Panel (b): The proton diagonal s.f. local density $\rho(q)$ shown as a function of the momentum transfer $q$ and the azimuthal angle $\theta$ for the excited state, $3^+$, of $^6\text{Li}$ ($N_{\text{max}} = 14$).

In summary, the $N_{\text{max}}$ of the NCSM calculation has a strong effect on the convergence of the binding energy of the nuclei, the shape of the space-fixed local density, and the contribution of the higher multipoles to the local density. For binding energy values and
local densities, the highest $N_{\text{max}}$ should be used to provide the best convergence possible. Though $N_{\text{max}} = 14$ is not a high enough value to see convergence on the binding energies and local densities of $^6\text{He}$ and $^6\text{Li}$, it can provide valuable insight into the expected shape of the ground and excited states of the nuclei.
4 TRANSLATIONALLY INVARIANT ONE-BODY DENSITIES FOR $^4$He, $^6$He, AND $^6$Li

The nuclear many-body Hamiltonian $H_A$, Eq. (3.1), introduced in the previous Section is Galilean invariant, and thus translationally invariant. However, the numerical solution of the many-body Schrödinger equation in the specific single particle basis of Slater determinants contains a fixed origin for the coordinate system. Thus, the many-body wave function contains a center-of-mass contribution. An experimental observable is always given as expectation value of a specific operator ‘sandwiched’ between wave functions of the system under consideration. Experimental observables like the matter radius, quadrupole moment of a nucleus, or its electromagnetic form factor are independent of the location of the experiment. Therefore, if a wave function that is used to compute those observables contains information about the c.m. of the system, the calculated observable can not be expected to describe the experiment.

For comparing calculated observables with measurements, it is necessary to obtain translationally invariant many-body wave functions. Dealing with the c.m. motion in many-body problems has a long history in nuclear structure theory [33, 34] and receives renewed interest when ab initio NCSM calculations of light nuclei are used to predict properties of stable and unstable nuclei [29, 35, 36].

The theoretical derivation that leads from a space-fixed to a translationally invariant (ti) local density is described in Section 4.1. Our calculations of the charge and matter radii of $^4$He, $^6$He, and $^6$Li are defined in Section 4.2 and the calculations of the form factors for those nuclei in Section 4.3, 4.4, and 4.5.
4.1 The Translationally Invariant Local One-Body Density

The many-body Hamiltonian $H_A$, Eq. (3.1), contains the single particle momenta $p_i$, and the single particle coordinates $r_i$, where $i = 1...A$. In general, a two-body interaction like the NN type depends only on the relative distance between the nucleons, $r = r_i - r_j$.

We can always define a total momentum of the system,

$$ P = \sum_{i=1}^{A} p_i, \quad (4.1) $$

which represents the c.m. momentum. The square of the sum of the single particle momenta as contained in the kinetic energy of the system can then be expressed as [18],

$$ \sum_{i=1}^{A} p_i^2 = \frac{1}{A} \left[ P^2 + \sum_{i<j} \left( p_i - p_j \right)^2 \right], \quad (4.2) $$

so that one obtains for the kinetic energy operator

$$ \left[ \sum_{i=1}^{A} \frac{p_i^2}{2m} - \frac{P^2}{2mA} \right] = \frac{1}{2mA} \sum_{i<j} \left( p_i - p_j \right)^2. \quad (4.3) $$

Defining a c.m. coordinate as

$$ R = \frac{1}{A} \sum_{i=1}^{A} r_i, \quad (4.4) $$

leads to

$$ \sum_{i=1}^{A} r_i^2 = \frac{1}{A} \left[ A^2 R^2 + \sum_{i<j} \left( r_i - r_j \right)^2 \right]. \quad (4.5) $$

Introducing Eqs. (4.2) and (4.5) into a HO one-body Hamiltonian

$$ H_{\text{one-body}} = \sum_{i=1}^{A} \left( \frac{p_i^2}{2m} + \frac{1}{2} m\Omega^2 r_i^2 \right), \quad (4.6) $$

where $\Omega$ is the HO frequency, leads to

$$ H_{HO} = \frac{P^2}{2mA} + \frac{mA\Omega^2 R^2}{2} + \frac{1}{2mA} \sum_{i<j} \left( p_i - p_j \right)^2 + \frac{m\Omega^2}{2A} \sum_{i<j} \left( r_i - r_j \right), \quad (4.7) $$

where the dependence on the c.m. coordinates is isolated in the first two terms,

$$ H_{c.m.} = \frac{P^2}{2mA} + \frac{mA\Omega^2 R^2}{2}. \quad (4.8) $$
A translationally invariant Hamiltonian for an A-nucleon system can be written as

\[ \hat{H} = \left[ \sum_{i=1}^{A} \frac{p_i^2}{2m} - \frac{P^2}{2mA} \right] + \sum_{i<j} V_{ij}. \]  

(4.9)

Adding a zero using Eq. (4.5),

\[ \sum_{i=1}^{A} \frac{1}{2} m \Omega^2 r_i^2 - \frac{m \Omega^2}{2A} \left[ A^2 \mathbf{R}^2 + \sum_{i<j}^{A} (\mathbf{r}_i - \mathbf{r}_j)^2 \right] = 0, \]  

(4.10)

allows the Hamiltonian to be rewritten as

\[ H = \sum_{i=1}^{A} \left[ \frac{p_i^2}{2m} + \frac{1}{2} m \Omega^2 r_i^2 \right] + \sum_{i<j}^{A} \left[ V_{ij} - \frac{m \Omega^2}{2A} (\mathbf{r}_i - \mathbf{r}_j)^2 \right] - H_{c.m.}, \]  

(4.11)

so that it is written in single particle coordinates, but still by construction translationally invariant. This feature is relevant for the numerical solution of the NCSM Hamiltonian.

The form of the Hamiltonian of Eq. (4.7) leads to another important insight. Schematically Eq. 4.11 can be written as

\[ H \Psi = (H_{\text{int}} + H_{c.m.}) \Psi = E \Psi, \]  

(4.12)

where the Hamiltonian that describes the intrinsic motion of the particles, \( H_{\text{int}} \), only depends on relative coordinates, while \( H_{c.m.} \) is given by Eq. (4.8). This form of the Hamiltonian suggests that the total wave function \( \Psi \) can be written as a product

\[ \Psi = \Psi_{\text{int}} \otimes \Phi_{c.m.}, \]  

(4.13)

with

\[ H_{\text{int}} \Psi_{\text{int}} = E_{\text{int}} \Psi_{\text{int}}, \]
\[ H_{c.m.} \Psi_{c.m.} = E_{c.m.} \Psi_{c.m.}, \]  

(4.14)

and

\[ E = E_{\text{int}} + E_{c.m.}. \]  

(4.15)

If one solves Eq. (4.11) in single particle coordinates in such a way that the c.m. is guaranteed to be in a 0s oscillator state, the intrinsic wave function and energy can be
obtained. When the single-particle levels of the oscillator potential are filled in their lowest energy state, the c.m. must also be in its lowest state 0s for the nucleus with mass $Am$ in the potential $\frac{1}{2}Am\Omega^2R^2$ with the c.m. energy

$$\langle \Psi | H_{c.m.} | \Psi \rangle = \frac{3}{2} \hbar \Omega \quad (4.16)$$

To ensure that the c.m. is in the 0s state, one can add a fictitious Hamiltonian, which only acts on the c.m. [34, 37],

$$H''_{c.m.} = \beta \left( \frac{P^2}{2mA} + \frac{1}{2}mA\Omega^2R^2 - \frac{3}{2} \hbar \Omega \right) \quad (4.17)$$

where the constant $\beta$ is made large enough so that the excitation energies of the c.m. are larger than all the intrinsic excitation energies of interest.

Having established in Eq. (4.13) that the total wave function can be written as a product, $\Psi_{int} \otimes \Phi_{c.m.}$, we can evaluate the c.m. piece explicitly, [38], as

$$\langle \mathbf{R} | \Phi_{c.m.,0s} \rangle = \Phi_{c.m.,0s}(\mathbf{R}) = \frac{2}{(b^2_{cm})^{3/4}} \frac{1}{\pi^{1/4}} e^{\frac{-b^2_{cm}}{4 \hbar \Omega}} \times \frac{1}{\sqrt{4\pi}} \quad (4.18)$$

with

$$b^2_{cm} = \frac{(hc)^2}{M^2 \hbar \Omega} = \frac{(hc)^2}{mA^2 \hbar \Omega} \quad (4.19)$$

Here we took advantage of Eqs. (3.2) and (3.4). The space-fixed local density is given in momentum space as

$$\langle \Psi_f J_f M_f | \rho(\mathbf{q}) | \Psi_i J_i M_i \rangle = \left\langle \Psi_f J_f M_f \left| \sum_n e^{-i\mathbf{q} \cdot \mathbf{r}_n} \right| \Psi_i J_i M_i \right\rangle \quad (4.20)$$

Employing relative coordinates, $z_n = \mathbf{r}_n - \mathbf{R}$, one obtains

$$\langle \Psi_f J_f M_f | \rho(\mathbf{q}) | \Psi_i J_i M_i \rangle = \left\langle \Psi_f J_f M_f \left| \sum_n e^{-i\mathbf{q} \cdot \mathbf{z}_n} e^{-i\mathbf{q} \cdot \mathbf{R}} \right| \Psi_i J_i M_i \right\rangle. \quad (4.21)$$
Using that $|\Psi_{iJM}\rangle = |\Psi_{int,JM}\rangle \otimes |\Phi_{cm,0s}\rangle$, 

$$
\left\langle \Psi_f J_f M_f | \rho(q) | \Psi_i J_i M_i \right\rangle = \left\langle \Phi_{cm,0s} | e^{-iqR} | \Phi_{cm,0s} \right\rangle \left\langle \Psi_{int,J_f M_f} \sum_n e^{-iqz_n} | \Psi_{int,J_i M_i} \right\rangle
$$

(4.22)

We can solve the c.m. matrix elements using Eq. (4.18) and arrive at

$$
\left\langle \Phi_{cm,0s} | e^{-iqR} | \Phi_{cm,0s} \right\rangle = e^{-\frac{q^2 b^2 cm}{4}}.
$$

(4.23)

Going back to Eq. (4.22) and defining

$$
\left\langle \Psi_{int,J_f M_f} \sum_n e^{-iqz_n} | \Psi_{int,J_i M_i} \right\rangle = \left\langle \Psi_{int,J_f M_f} | \rho_{ti}(q) | \Psi_{int,J_i M_i} \right\rangle,
$$

(4.24)

we arrive at

$$
\left\langle \Psi_f J_f M_f | \rho(q) | \Psi_i J_i M_i \right\rangle = \left\langle \Phi_{cm,0s} | e^{-iqR} | \Phi_{cm,0s} \right\rangle \left\langle \Psi_{int,J_f M_f} \sum_n e^{-iqz_n} | \Psi_{int,J_i M_i} \right\rangle
$$

$$
= e^{-\frac{q^2 b^2 cm}{4}} \left\langle \Psi_{int,J_f M_f} \rho_{ti}(q) | \Psi_{int,J_i M_i} \right\rangle,
$$

(4.25)

which leaves us with

$$
\left\langle \Psi_{int,J_f M_f} | \rho_{ti}(q) | \Psi_{int,J_i M_i} \right\rangle = e^{\frac{q^2 b^2 cm}{4}} \left\langle \Psi_f J_f M_f | \rho(q) | \Psi_i J_i M_i \right\rangle
$$

$$
= e^{\frac{q^2 b^2}{4\pi}} \left\langle \Psi_f J_f M_f | \rho(q) | \Psi_i J_i M_i \right\rangle.
$$

(4.26)

From Eq. (4.26) we can compute the translationally invariant momentum space density matrix elements and, using an inverse fourier transform, the position space elements as well.

### 4.2 Point and Charge Radii

The root-mean-square (RMS) radius is a quantity that must be calculated in the translationally invariant (t.i.) frame, and can be expressed as

$$
\langle r^2 \rangle^{1/2} = \left[ \frac{\int \rho(r) r^2 d^3r}{\int \rho(r) d^3r} \right]^{1/2} = \sqrt{\left\langle \Psi_{ti} | r^2 | \Psi_{ti} \right\rangle}.
$$

(4.27)

An important note is that the radii obtained from using Eq. (4.27), using our local densities, are the point radii. These values cannot be compared to experiment because they
have the assumption that protons and neutrons are point-like particles. Thus, the calculated point-proton radius must be converted to the charge radius when comparing with experimental results, such as those obtained from isotope shifts of atomic x-ray transitions. The relation to convert from the point-proton radius to the charge radius is

\[ R_p = \sqrt{R_{ch}^2 - R_{op}^2 - \frac{N}{Z} R_{on}^2 + R_{rel}^2}, \]  

(4.28)

according to Ref. [39] where \( R_{op}^2 \) is the mean-square radius of the proton, \( R_{on} = -0.1161(22) \) fm\(^2\) is the mean-square radius of the neutron, and \( R_{rel}^2 = 0.033 \) fm\(^2\) is a Darwin-Foldy relativistic correction of first-order. The value of \( R_p \), according to the Review of Particle Physics [40], is 0.877(7) fm. There are smaller correction terms that can be included to get a more accurate comparison between the two radii [39]. The point-matter radius is calculated by the combined proton and neutron densities after removal of the center of mass, \( \langle r_m^2 \rangle^{1/2} = \left\langle |\Psi_{p,t,i} + \Psi_{n,t,i}|^2 \right\rangle \left| \Psi_{p,t,i} + \Psi_{n,t,i} \right\rangle \). The point-matter radius and point-neutron radius computed in this work are not compared to experimental values and do not need to be converted in later Sections.

### 4.3 Translationally Invariant Local Density for \(^4\)He

In this Section, the point-proton, point-neutron, and point-matter radii along with the translationally invariant two-dimensional (2D) local density are calculated and shown for the nucleus \(^4\)He with the \( N_{max} = 14 \) data set [30]. As before, the data files contain separate coefficients for the proton and neutron density distributions, and thus they are separately reconstructed. In the calculation of \(^4\)He, the Coulomb interaction between the protons is neglected and thus the proton and neutron local densities are identical, therefore only the proton distributions are shown. In Table 4.1, the point radii are given for the proton, neutron, and matter densities. The point matter radius is calculated using Eq. (4.27) and a sum of the neutron and proton local densities after removal of the center of mass for each.
Table 4.1: The point-proton, point-neutron, and point-matter radii, Eq. (4.27), for $^4\text{He}$. The order of the states, top to bottom, show the order of excitation energy levels. The calculations are based on a $N_{\text{max}} = 14$ NCSM calculation [30], which neglects the Coulomb interaction between the protons.

<table>
<thead>
<tr>
<th>State</th>
<th>Proton</th>
<th>Neutron</th>
<th>Matter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0^+_1 \text{ g.s.}$</td>
<td>1.42(593587)</td>
<td>1.42(604334)</td>
<td>1.42(598960)</td>
</tr>
<tr>
<td>$0^+_2$</td>
<td>2.61(051893)</td>
<td>2.61(065539)</td>
<td>2.61(058716)</td>
</tr>
<tr>
<td>$1^-_1$</td>
<td>2.94(256768)</td>
<td>2.94(254520)</td>
<td>2.94(255644)</td>
</tr>
<tr>
<td>$1^-_2$</td>
<td>2.95(264022)</td>
<td>2.95(266226)</td>
<td>2.95(265124)</td>
</tr>
<tr>
<td>$0^+_3$</td>
<td>2.98(588264)</td>
<td>2.98(588267)</td>
<td>2.98(588265)</td>
</tr>
</tbody>
</table>

After converting the ground state point-proton radius from the $^4\text{He}$ calculations to the charge radius using Eq. (4.28), we arrive at a charge radius $R_{\text{ch}} = 1.649$ fm for the ground state. Comparing this with the value by Ingo Sick [41], of $1.681 \pm 0.004$ fm, we can see that our result slightly underestimates the experimental value. Our calculation does not include the Coulomb interaction between protons so when that information is added to the computation, we should expect our charge radius to move closer to the experimental result.

In Fig. 4.1, the space-fixed (s.f.) and translationally invariant (t.i.) local density is shown for the ground state of $^4\text{He}$, computed from the $N_{\text{max}} = 14$ data files, as a function of the distance $r$ from the c.m. and the momentum transfer $q$. In panel (b), the momentum space local density distributions are multiplied by $Y^0_0(\theta, \phi)$ to insure the normalization $\rho(0)(q = 0) = A$. The center of mass removal from the ground state of $^4\text{He}$ causes a large increase of the local density at high $q$ values ($2 \text{ fm}^{-1}$ and further) which translates to a more compact position space density that has a larger magnitude at low $r$ but falls off more quickly at higher $r$ values. The dramatic increase in panel (b) of Fig. 4.1 shows that it is imperative to calculate physical observables with t.i. densities.
Figure 4.1: The diagonal space-fixed local density $\rho^{(0)}(r)$ and $\rho^{(0)}(q)$ of the ground state, $0^+$, for $^4$He ($N_{\text{max}} = 14$). Panel (a) shows the coordinate space density, while panel (b) depicts the momentum space density, with $\rho^{(0)}(q)$ multiplied by $Y_0^0(\hat{q})$.

The t.i. local density for the $1^-$ excited state of $^4$He, computed from the $N_{\text{max}} = 14$ data set, is shown in Fig. 4.2 along with the s.f. density for comparison. The $K=0$ part of the momentum space local density, panel (b), is multiplied by $Y_0^0(\theta, \phi)$ to insure the normalization $\rho^{(0)}(q = 0) = A$. The $K=2$ pieces of the excited state in Fig. 4.2 are multiplied by a factor of 20 to increase the visibility of the features. The c.m. removal only affects the $K=0$ piece of the local density, thus the s.f. $K=2$ multipole is not shown.

The most obvious effect of the c.m. removal on the excited state $1^-$ is the extension of the $K=0$ multipole in momentum space with the slight dip into negative values around 2.3 fm$^{-1}$ and beyond. These negative values in the momentum space translate into the shape of the t.i. local density towards low $r$ in position space. The increase of the local density in momentum space before 2.3 fm$^{-1}$ causes the position space density to fall off more quickly at higher $r$ values. Such a change on the local density should lower the radius because of the larger contribution higher $r$ values have in the calculation. Since the c.m.
removal process does not affect the density along the \( \theta \) axis, we do not need to show the comparison between the s.f. and t.i. local density in 3D.

Figure 4.2: The diagonal space-fixed local density \( \rho^{(K)}(r)C_K \) and \( \rho^{(K)}(q)C_K \) of the \( 1^- \) excited state of \( ^4\text{He} \) (\( N_{\text{max}} = 14 \)). Panel (a) gives the coordinate space density with \( \rho^{(2)}(r) \) multiplied by a factor of 20. Panel (b) depicts the momentum space density with \( \rho^{(0)}(q) \) multiplied by the \( Y_0^0(\hat{q}) \) and \( \rho^{(2)}(q) \) is multiplied by a factor of 20.

4.4 Translationally Invariant Local Density for \( ^6\text{He} \)

In this Section the point radius and the translationally invariant two-dimensional (2D) local density are calculated and shown for the nucleus \( ^6\text{He} \) with the \( N_{\text{max}} = 14 \) data set [30]. As before, the data files contain separate coefficients for the proton and neutron density distributions, and thus they are separately reconstructed. In Table 4.2, the point radii are given for the proton, neutron, and matter densities. Immediately after comparing the radii with those from the \( ^4\text{He} \) calculation, it is apparent that the addition of 2 neutrons causes both the radius of the neutrons and the protons to increase.
Table 4.2: The point-proton, point-neutron, and point-matter radii, Eq. (4.27), for $^6$He. The order of the states, top to bottom, show the order of excitation energy levels. The calculations are based on a $N_{max} = 14$ NCSM calculation [30], which neglects the Coulomb interaction between the protons.

<table>
<thead>
<tr>
<th>State</th>
<th>Proton</th>
<th>Neutron</th>
<th>Matter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0^+_1$ g.s.</td>
<td>1.39(993491)</td>
<td>2.27(174340)</td>
<td>2.02(331048)</td>
</tr>
<tr>
<td>$2^+_1$</td>
<td>1.38(439197)</td>
<td>2.35(594007)</td>
<td>2.08(304725)</td>
</tr>
<tr>
<td>$2^+_2$</td>
<td>1.46(803497)</td>
<td>2.62(838580)</td>
<td>2.30(734825)</td>
</tr>
<tr>
<td>$1^-$</td>
<td>1.47(983970)</td>
<td>2.72(858771)</td>
<td>2.38(605990)</td>
</tr>
<tr>
<td>$0^+_2$</td>
<td>1.58(503367)</td>
<td>2.83(334019)</td>
<td>2.48(781444)</td>
</tr>
</tbody>
</table>

After converting the ground state point-proton radius from the $^6$He calculations to the charge radius using Eq. (4.28), we arrive at a charge radius $R_{ch} = 1.591$ fm for the ground state. Comparing this with the value reported in 2012 by Bacca et al. [39] of $R_{ch} = 2.060 \pm 0.008$ fm, we can see that our result does not fall within the experimental error. Our calculation does not include the Coulomb interaction between protons so when that piece is added to the computation, we should expect our charge radius to move towards the experimental result.

In Fig. 4.3, the space-fixed (s.f.) and translationally invariant (t.i.) local densities are shown for the ground state of $^6$He’s neutrons, computed from the $N_{max} = 14$ data files, as a function of the distance $r$ from the c.m. and the momentum transfer $q$. In panel (b), the momentum space local density distributions are multiplied by $Y^0_0(\theta, \phi)$ to insure the normalization $\rho^{(0)}(q = 0) = A$. The center of mass removal from the ground state of $^6$He causes a modest increase of the local density at $q$ values higher than about 1 fm$^{-1}$ which translates to a more compact position space density that has a larger magnitude at low $r$ but falls off a little more quickly at higher $r$ values. The result of removing the c.m. is that the radius should become smaller.
Figure 4.3: The neutron t.i. and s.f. local densities $\rho^{(0)}(r)$ and $\rho^{(0)}(q)$ of the ground state, $0^+$, for $^6$He ($N_{\text{max}} = 14$). Panel (a) shows the coordinate space density, while panel (b) depicts the momentum space density, with $\rho^{(0)}(q)$ multiplied by $Y_0^0(\hat{q})$.

In Fig. 4.4, the s.f. and t.i. local density is shown for the ground state of $^6$He’s protons, computed from the $N_{\text{max}} = 14$ data files, as a function of the distance $r$ from the c.m. and the momentum transfer $q$. In panel (b), the momentum space local density distributions are multiplied by $Y_0^0(\theta, \phi)$ to insure the normalization $\rho^{(0)}(q = 0) = A$. The center of mass removal from the ground state of $^6$He for the proton local density causes a slower fall off of the local density at $q$ values higher than the origin. This slower fall off translates to a compact position space density that has a larger magnitude at low $r$ but falls off a little more quickly at higher $r$ values.

The large difference in effect that removing the c.m. has on $^6$He’s protons versus its neutrons is due to the increase in number of nucleons involved in the c.m. contribution. When the c.m. is removed for the protons, using Eq. (4.26), $A = 2$ and the increase of the c.m. contribution along the $q$-axis is large. However, when the c.m. is removed for the neutrons $A = 4$, the exponential in Eq. (4.26) is diminished immensely. To illustrate this
fact more clearly, Table 4.3 shows when the exponential in Eq. (4.26) approaches the value ‘5’ when increasing $q$.

Table 4.3: The $q$ values for which $e^{q b^2 / A} = 5$, using Eq. (4.26) for different $A$ values. The value of $b$ is taken to be 2 in this example.

<table>
<thead>
<tr>
<th>$A$</th>
<th>$q$</th>
<th>$e^{q b^2 / A}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.794</td>
<td>5.0</td>
</tr>
<tr>
<td>3</td>
<td>2.197</td>
<td>5.0</td>
</tr>
<tr>
<td>4</td>
<td>2.537</td>
<td>5.0</td>
</tr>
<tr>
<td>6</td>
<td>3.108</td>
<td>5.0</td>
</tr>
<tr>
<td>8</td>
<td>3.588</td>
<td>5.0</td>
</tr>
</tbody>
</table>

Figure 4.4: The proton t.i. and s.f. local densities $\rho^{(0)}(r)$ and $\rho^{(0)}(q)$ of the ground state, $0^+$, for $^6$He ($N_{\text{max}} = 14$). Panel (a) shows the coordinate space density, while panel (b) depicts the momentum space density, with $\rho^{(0)}(q)$ multiplied by $Y_0^0(\hat{q})$.
The neutron t.i. local density for the $2^+$ excited state of $^6$He, computed from the $N_{\text{max}} = 14$ data set, is shown in Fig. 4.5 along with the s.f. density for comparison. The $K=0$ part of the momentum space local density, panel (b), is multiplied by $Y_0^0(\theta, \phi)$ to insure the normalization $\rho^{(0)}(q = 0) = A$. The $K=2$ pieces of the excited state in Fig. 4.2 are multiplied by a factor of 5 to increase its visibility. The s.f. $K=2$ multipole is not shown because the c.m. removal only affects the $K=0$ piece of the local density. The effect of the c.m. removal is an extension towards higher $q$ of the $K=0$ multipole in momentum space. The increase of the local density in momentum space causes the position space density to fall off more sharply at higher $r$ values while having a higher magnitude near the origin. The radius is expected to decrease.

Figure 4.5: The neutron t.i. and s.f. local densities $\rho^{(K)}(r)C_K$ and $\rho^{(K)}(q)C_K$ of the $2^+$ excited state of $^6$He ($N_{\text{max}} = 14$). Panel (a) gives the coordinate space density with $\rho^{(2)}(r)$ multiplied by a factor of 5. Panel (b) depicts the momentum space density with $\rho^{(0)}(q)$ multiplied by $Y_0^0(\hat{q})$ and $\rho^{(2)}(q)$ is multiplied by a factor of 5.
The proton t.i. local density for the $2^+$ excited state of $^6$He, computed from the $N_{\text{max}} = 14$ data set, is shown in Fig. 4.6 along with the s.f. density for comparison. The $K=0$ part of the momentum space local density, panel (b), is multiplied by $Y_0^0(\theta, \phi)$ to insure the normalization $\rho^{(0)}(q = 0) = A$. The $K=2$ pieces of the excited state in Fig. 4.6 are multiplied by a factor of 20 to increase their visibility. The c.m. removal only affects the $K=0$ piece of the local density, thus the s.f. $K=2$ multipole is not shown. Just like the ground state, the effect of the c.m. removal is more prominent in the proton density than the neutron one. The extension of the $K=0$ multipole in momentum space causes the position space density to fall off more sharply at higher $r$ values while having a higher magnitude near the origin. Since the c.m. removal process does not affect the density along the $\theta$ axis, we do not need to show the comparison between the s.f. and t.i. local density in 3D.

Figure 4.6: The proton t.i. and s.f. local densities $\rho^{(K)}(r)C_K$ and $\rho^{(K)}(q)C_K$ of the $2^+$ excited state of $^6$He ($N_{\text{max}} = 14$). Panel (a) gives the coordinate space density with $\rho^{(2)}(r)$ multiplied by a factor of 20. Panel (b) depicts the momentum space density with $\rho^{(0)}(q)$ multiplied by $Y_0^0(\hat{q})$ and $\rho^{(2)}(q)$ is multiplied by a factor of 20.
4.5 Translationally Invariant Local Density for $^6\text{Li}$

In this Section the point radius and the translationally invariant two-dimensional (2D) local density are calculated and shown for the nucleus $^6\text{Li}$ with the $N_{\text{max}} = 14$ data set [30]. As before, the data files contain separate coefficients for the proton and neutron density distributions, and thus they are separately reconstructed. In this calculation of $^6\text{Li}$, the Coulomb interaction between the protons is neglected and thus the proton and neutron local densities are identical, therefore only proton distributions are shown. In Table 4.4, the point radii are given for the proton, neutron, and matter densities.

Table 4.4: The point-proton, point-neutron, and point-matter radii, Eq. (4.27), for $^6\text{Li}$. The order of the states, top to bottom, show the order of excitation energy levels. The calculations are based on a $N_{\text{max}} = 14$ NCSM calculation [30], which neglects the Coulomb interaction between the protons.

<table>
<thead>
<tr>
<th>State</th>
<th>Proton</th>
<th>Neutron</th>
<th>Matter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1^+$ g.s.</td>
<td>2.00(837013)</td>
<td>2.00(837011)</td>
<td>2.00(837012)</td>
</tr>
<tr>
<td>$3^+$</td>
<td>1.94(741285)</td>
<td>1.94(741293)</td>
<td>1.94(741289)</td>
</tr>
<tr>
<td>$0^+$</td>
<td>2.02(351153)</td>
<td>2.02(351155)</td>
<td>2.02(351154)</td>
</tr>
<tr>
<td>$2^+_1$</td>
<td>2.12(088376)</td>
<td>2.12(088376)</td>
<td>2.12(088376)</td>
</tr>
<tr>
<td>$2^+_2$</td>
<td>2.08(357201)</td>
<td>2.08(357214)</td>
<td>2.08(357207)</td>
</tr>
</tbody>
</table>

After converting the ground state point-proton radius from the $^6\text{Li}$ calculations to the charge radius using Eq. (4.28), we arrive at a charge radius $R_{\text{ch}} = 2.172$ fm for the ground state. Comparing this with the value found by Ingo Sick [41] of $R_{\text{ch}} = 2.589 \pm 0.039$ fm, we can see that our result underestimates the experimental value. However, our calculation does not include the Coulomb interaction between protons so when that piece is included, we should expect our result to move closer to the reported value.
In Fig. 4.7, the space-fixed (s.f.) and translationally invariant (t.i.) local densities are shown for the ground state 1+ of $^6$Li’s protons, computed from the $N_{\text{max}} = 14$ data files, as a function of the distance $r$ from the c.m. and the momentum transfer $q$. In panel (b), the momentum space local density distributions are multiplied by $Y_0^0(\theta, \phi)$ to insure the normalization $\rho^{(0)}(q = 0) = A$. The $K=2$ pieces of the excited state in Fig. 4.7 are multiplied by a factor of 5 to increase the visibility of the features. The c.m. removal only affects the $K=0$ piece of the local density, thus the s.f. $K=2$ multipole is not shown. The center of mass removal from the ground state of $^6$Li causes a modest increase of the local density at $q$ values higher than about 1 fm$^{-1}$. This slower fall off in momentum space translates to a more compact position space density that has a larger magnitude at low $r$ but falls off a little more quickly at higher $r$ values. The result of such a change is that the radius should be smaller than the non-c.m.-removed local density.

Figure 4.7: The proton t.i. local density $\rho^{(K)}(r)C_K$ and $\rho^{(K)}(q)C_K$ of the ground state, 1+, for $^6$Li ($N_{\text{max}} = 14$). Panel (a) shows the coordinate space density with $\rho^{(2)}(r)$ multiplied by a factor of 5, while panel (b) depicts the momentum space density with $\rho^{(0)}(q)$ multiplied by $Y_0^0(\hat{q})$ and $\rho^{(2)}(q)$ is multiplied by a factor of 5.
In Fig. 4.8, the s.f. and t.i. local density is shown for the excited state $3^+$ of $^6$Li’s protons, computed from the $N_{\text{max}} = 14$ data files, as a function of the distance $r$ from the c.m. and the momentum transfer $q$. In panel (b), the momentum space local density distributions are multiplied by $Y_0^0(\theta, \phi)$ to insure the normalization $\rho^{(0)}(q = 0) = A$. The $K = 2$ pieces of the excited state in Fig. 4.8 are multiplied by a factor of 5 to increase the visibility of the features. The c.m. removal only affects the $K = 0$ piece of the local density, thus the s.f. $K = 2$ multipole is not shown. The center of mass removal from the excited state of $^6$Li has the same effect as on the ground state, namely a slower fall off in momentum space and faster fall off in position space with a higher magnitude at the origin $r = 0$. Similarly, the result of such a change in the local densities is that the radius should be smaller after removing the center of mass. Since the c.m. removal process does not affect the density along the $\theta$ axis, we do not need to show the comparison between the s.f. and t.i. local density in 3D.
Figure 4.8: The proton t.i. local density $\rho^{(K)}(r)C_K$ and $\rho^{(K)}(q)C_K$ of the excited state, $3^+$, for $^6\text{Li}$ ($N_{\text{max}}=14$). Panel (a) shows the coordinate space density with $\rho^{(2)}(r)$ multiplied by a factor of 5, while panel (b) depicts the momentum space density with $\rho^{(0)}(q)$ multiplied by $Y_0^0(\hat{q})$ and $\rho^{(2)}(q)$ is multiplied by a factor of 5.

In summary, the center of mass contribution to the local densities of light, $A=2$, nuclei is quite dramatic. Once the center of mass effect is removed then observables of the system can be calculated and compared to experimental values. For very heavy nuclei, from the results shown here, we expect to see a very small contribution of the center of mass to the local densities and observables. Though the Coulomb interaction was not included in the NCSM calculation inputs, the resulting root-mean-square radii have potential to move closer to experimental values with higher $N_{\text{max}}$ values and the inclusion of the interaction in the Hamiltonian.
5SUMMARY AND OUTLOOK

This work completed NCSM calculations of translationally invariant local densities for $^4\text{He}$, $^6\text{He}$, and $^6\text{Li}$. Along the way, the M-Scheme for setting up a many-body basis was discussed. A simple example Hamiltonian was given in Chapter 2 so that the Maris-Vary one-body-density-matrix-elements used in Chapter 3 could be more easily understood. Chapter 3 went through all relevant calculations to obtain a space-fixed local density for each of the nuclei with explicit derivations for the radial piece of the wave function given in Appendix A and the associated numerical checks shown in Appendix C. When the translationally-invariant local density was introduced in Chapter 4, we discussed how the removal of the center-of-mass contribution is imperative for extracting observables from the system. It was also shown how only in a Harmonic Oscillator basis can the center-of-mass be removed exactly. The radii given in the same Chapter after the removal of the center-of-mass give a comparison from this work’s calculations and the experimental values for each nucleus.

This work has many different possible avenues for future research. One of the first and most obvious continuations of this work is to use a slightly more realistic Hamiltonian that includes the Coulomb interaction between the protons of the system. This will allow a more realistic comparison between the NCSM calculation and experiment, even if the $N_{\text{max}}$ data set is not converged. Another possible continuation of this work will be to perform the removal of the center-of-mass in position space, which has been carried out in Ref. [35], to compare with the removal completed in momentum space that is performed here. Related, the calculation of the local density may be performed directly in momentum space. This change in computation would reduce the numerical errors by removing the Fourier transform from position space to momentum space. Even further down the road will be computing the non-local density, where the initial and final states are not the same. This will lead directly into calculation of microscopic optical potentials...
based on NCSM structure information for proton and neutron elastic scattering, a goal for a future PhD thesis.
REFERENCES


[37] B. A. Brown, Lecture Notes in Nuclear Structure Physics (NSCL and Department of Physics and Astronomy, Michigan State University, E. Lansing, MI 48824, 2005).

[38] K. Launey, (private communication).


APPENDIX A: DERIVATION OF THE RADIAL FUNCTION OF THE

THREE-DIMENSIONAL HARMONIC OSCILLATOR

This Appendix gives the explicit derivation of the radial function for the
three-dimensional harmonic oscillator potential. We start from the general product ansatz
for the wave function for which the potential exhibits rotational symmetry,

\[ \psi_{nlm}(r, \theta, \phi) = R_{nl}(r) \Phi_{lm}(\theta, \phi) \]  \hspace{1cm} (A.1)

The \( R_{nl}(r) \) term describes the radial dependence of the wave function while the \( \Phi_{lm}(\theta, \phi) \) term contains the angular dependence. After separating the angular and radial
contributions, the radial wave functions fulfills

\[ -\frac{\hbar^2}{2m r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} R_{nl}(r) \right) + \left[ \frac{\hbar^2}{2m \hbar \Omega} \frac{l(l+1)}{r^2} + \frac{1}{2} \frac{m \Omega^2}{\hbar} r^2 \right] R_{nl}(r) = E R_{nl}(r) \]  \hspace{1cm} (A.2)

Dividing both sides by \( \hbar \Omega \) and defining \( \epsilon = \frac{E}{\hbar \Omega} \), one obtains

\[ -\frac{\hbar^2}{2m \hbar \Omega r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} R_{nl}(r) \right) + \left[ \frac{\hbar^2}{2m \hbar \Omega} \frac{l(l+1)}{r^2} + \frac{1}{2} \frac{m \Omega^2}{\hbar} r^2 \right] R_{nl}(r) = \frac{E}{\hbar \Omega} R_{nl}(r) \]  \hspace{1cm} (A.3)

Defining \( b = \sqrt{\frac{\hbar}{m \Omega}} \) leads to

\[ -\frac{\hbar}{2m \Omega} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} R_{nl}(r) \right) + \left[ \frac{\hbar}{2m \Omega} \frac{l(l+1)}{r^2} + \frac{1}{2} \frac{m \Omega^2}{\hbar} r^2 \right] R_{nl}(r) = \epsilon R_{nl}(r) \]  \hspace{1cm} (A.4)

Replacing the dimensionless quantity \( \frac{r}{b} \) with \( q \) leads to \( \frac{d}{dr} = \frac{1}{b} \frac{dq}{dr} \). Thus the result is

\[ \frac{1}{q^2} \frac{d}{dq} \left( q^2 \frac{d}{dq} R_{nl}(q) \right) - \left[ \frac{l(l+1)}{q^2} + q^2 \right] R_{nl}(q) = -2\epsilon R_{nl}(q) \]  \hspace{1cm} (A.5)

Now we want to consider the physical boundary conditions. The first boundary to look at
is \( q \to 0 \),
We assume a form $R(q) = q^\alpha f(q)$. Thus,

$$
\frac{1}{q^2} \frac{d}{dq} \left( q^2 \frac{d}{dq} q^\alpha f(q) \right) - \left[ \frac{l(l+1)}{q^2} + q^\alpha \right] q^\alpha f(q) = -2\varepsilon q^\alpha f(q)
$$

and

$$
\frac{1}{q^2} \frac{d}{dq} q^2 \left( aq^{\alpha-1} f + q^\alpha \frac{df}{dq} \right) - \left[ \frac{l(l+1)}{q^2} + q^\alpha \right] q^\alpha f = -2\varepsilon q^\alpha f
$$

The coefficient of $q^{\alpha-2} f$ must be zero in order to match the right side. We know that $q^{\alpha-2}$ and $f$ are not zero. Thus,

$$\alpha(\alpha + 1) = l(l + 1). \quad (A.7)$$

The only solutions are $l = \alpha$ or $l = -\alpha - 1$. We can rule out $-\alpha - 1$ as solution. This leads to the differential equation

$$
(2l + 2)q^{l+1} \frac{df}{dq} + q^l \frac{d^2 f}{dq^2} - q^{l+2} f + 2\varepsilon q^l f = 0. \quad (A.8)
$$

Now we divide by $q^l$, set $q^2 = z$ and let $f(q) \to v(q)$. This means we need to make the substitutions

$$
q = \sqrt{z} \quad \frac{d}{dq} = 2 \sqrt{z} \frac{d}{dz} \quad \frac{d^2}{dq^2} = 2 \sqrt{z} \frac{d}{dz} (2 \sqrt{z} \frac{d}{dz}) = 2 \frac{d}{dz} + 4z \frac{d^2}{dz^2}, \quad (A.9)
$$

and thus the differential equation becomes

$$
\frac{d^2 f}{dq^2} + (2l + 2)q^{-l-1} \frac{df}{dq} + [2\varepsilon - q^2] f = 0
$$

$$
2 \frac{dv}{dz} + 4z \frac{d^2 v}{dz^2} + (2l + 2)z^{-l-1} 2z \frac{dv}{dz} + [2\varepsilon - z] v = 0
$$

$$
v'' + 2l + 3 \frac{v'}{2z} + \frac{2\varepsilon - z}{4z} v = 0 \quad (A.10)
$$
The other boundary condition requires $v \to 0$ as $z \to \infty$. Thus,

$$v'' + 0 + \left[ 0 - \frac{1}{4} \right] v = 0$$

$$v'' = \frac{1}{4} v$$

$$v = C(z)e^z + w(z)e^{-z}. \quad (A.11)$$

Since $v = C(z)e^z$ will diverge as $z \to \infty$ we choose

$$v = w(z)e^{-z}$$

$$v' = \left[ w' - \frac{w}{2} \right] e^{-z}$$

$$v'' = \left[ w'' - \frac{1}{2}w' - \frac{1}{2}w' + \frac{1}{4}w \right] e^{-z}$$

$$v'' = \left[ w'' - w' + \frac{w}{4} \right] e^{-z}. \quad (A.12)$$

Inserting everything back into Eq. (A.10) and dividing out the term $e^{-z}$ leads to

$$v'' + \frac{2l + 3}{2z} v' + \frac{2\epsilon - z}{4z} v = 0$$

$$\left[ w'' - w' + \frac{w}{4} \right] + \frac{2l + 3}{2z} \left[ w' - \frac{w}{2} \right] + \frac{2\epsilon - z}{4z} w = 0$$

$$zw'' + w' \left[ l + \frac{3}{2} - z \right] + w \left[ \epsilon - l - \frac{3}{2} \right] \frac{1}{2} = 0. \quad (A.13)$$

Kummer’s equation has the form $xy'' + (c - x)y' - ay = 0$. The solution is $y =_1 F_1(a; c; x)$, where $_1F_1$ is the Confluent Hyper-geometric Function of the first kind. The function

$$_1F_1(a; c; x)$$

can be related to the Associated Laguerre Polynomials via

$$_1F_1(-n; \alpha + 1; x) = \frac{n!}{(\alpha + 1)_n} L_n^{(\alpha)}(x)$$

$$_1F_1(-n; \alpha + 1; x) = \frac{n!\alpha!}{(\alpha + n)!} L_n^{(\alpha)}(x) \quad (A.14)$$

Thus, with the current form of Eq. (A.13) we have

$$w = _1F_1\left(\frac{1}{2}(\epsilon - l - \frac{3}{2}); (l + \frac{3}{2}); z\right)$$

$$w = \frac{(\frac{1}{2}(\epsilon - l - \frac{3}{2}))!(l + \frac{1}{2})!}{(l + \frac{1}{2} + \frac{1}{2}(\epsilon - l - \frac{3}{2}))!} L_{\frac{1}{2}}^{l+\frac{1}{2}}(\epsilon - l - \frac{1}{2})(z)$$

$$w(z) = \frac{n!(l + \frac{1}{2})!}{(l + \frac{1}{2} + n)!} L_n^{l+\frac{1}{2}}(z). \quad (A.15)$$
Relating back to $R_{nl}(r)$ for the radial solution of the 3D harmonic oscillator

\[ q^2 = z = \frac{r^2}{b^2} \]

\[ R_{nl}(r) = N_{nl} q^{\frac{1}{2}} f(q) = N_{nl} z^{\frac{1}{2}} v(z) \]

\[ v(z) = w(z)e^{-\frac{z}{2}} \]

\[ R_{nl}(r) = N_{nl} \left( \frac{r^2}{b^2} \right)^{\frac{1}{2}} w\left( \frac{r^2}{b^2} \right) e^{-\frac{r^2}{2b^2}} \]

\[ R_{nl}(r) = N_{nl} \left( \frac{r^2}{b^2} \right)^{\frac{1}{2}} e^{-\frac{r^2}{2b^2}} \frac{n!(l + \frac{1}{2})!}{(l + \frac{1}{2} + n)!} \frac{n!(l + \frac{1}{2})!}{L_{n}^{l+\frac{1}{2}} \left( \frac{r^2}{b^2} \right)} . \quad (A.16) \]

For the normalization factor $N_{nl}$ we refer to outside sources [42] and confirm with a numerical check given in Appendix [C]. From Ref. [42] we get

\[ N_{nl} = \frac{1}{b^{3/2}} \sqrt{\frac{2}{\Gamma(n + l + \frac{3}{2})}} \frac{\Gamma(n + 1)}{\Gamma(l + \frac{3}{2})} \]  

\[ (A.17) \]

Inserting Eq. (A.17) into Eq. (A.16) we arrive at our final expression for the radial wave function of the 3D Harmonic Oscillator,

\[ R_{nl}(r) = N_{nl} \left( \frac{r^2}{b^2} \right)^{\frac{1}{2}} e^{-\frac{r^2}{2b^2}} \frac{n!(l + \frac{1}{2})!}{(l + \frac{1}{2} + n)!} \frac{n!(l + \frac{1}{2})!}{L_{n}^{l+\frac{1}{2}} \left( \frac{r^2}{b^2} \right)} \]

\[ R_{nl}(r) = \frac{1}{b^{3/2}} \sqrt{\frac{2}{\Gamma(n + l + \frac{3}{2})}} \frac{\Gamma(n + 1)}{\Gamma(l + \frac{3}{2})} \left( \frac{r^2}{b^2} \right)^{\frac{1}{2}} \frac{n!(l + \frac{1}{2})!}{(l + \frac{1}{2} + n)!} \frac{n!(l + \frac{1}{2})!}{L_{n}^{l+\frac{1}{2}} \left( \frac{r^2}{b^2} \right)} \]

\[ R_{nl}(r) = \frac{1}{\sqrt{\Gamma(l + \frac{3}{2} + n)}} \frac{\Gamma(n + 1)}{2b^2} \left( \frac{r^2}{b^2} \right)^{l+\frac{1}{2}} L_{n}^{l+\frac{1}{2}} \left( \frac{r^2}{b^2} \right) . \quad (A.18) \]

One can define $\nu = \frac{mc^2}{2\hbar^2}$, in which case the final expression for the radial wave function becomes

\[ R_{nl}(r) = \sqrt{\frac{2}{\Gamma(l + \frac{3}{2} + n)}} \frac{(2\nu)^{l+\frac{1}{2}} \Gamma(n + 1)}{2\nu} \frac{r^2 e^{-\nu r^2} L_{n}^{l+\frac{1}{2}} \left( 2\nu r^2 \right)} . \quad (A.19) \]

This result agrees with Eqs. (1.39) and (1.41) in Chase Cockrell’s Thesis [43]. However, Eq. (2.21) in the thesis and Eq. (A13) in the appendix of Ref. [29] are incorrect and do not correspond to this result.
APPENDIX B: DERIVATION OF THE K=0, 1, AND 2 MULTIPOLAR TERMS OF THE SPACE-FIXED LOCAL DENSITY

In this Appendix, the explicit derivations of the K=0, 1, and 2 multipole terms are carried out for the space-fixed local density.

B.1 Derivations of the K=0 Multipole Term

In this Section we calculate the zeroth multi-pole of the coordinate space density. Beginning with Eq. (3.11),

\[ \rho_{sf}^{(K)}(r) = \sum R_{n_1 l_1}(r) R_{n_2 l_2}(r) \frac{-1}{\sqrt{2K+1}} \int \frac{l_1}{2} j_1 \|Y_K\| \frac{l_2}{2} j_2 \langle A J A \| (a^+_{n_1 l_1 j_1} \tilde{a}_{n_2 l_2 j_2})^{(K)} \| A J A \rangle \]  

(B.1)

Setting K = 0 leads to

\[ \rho_{sf}^{(0)}(r) = \sum R_{n_1 l_1}(r) R_{n_2 l_2}(r) \frac{-1}{1} \int \frac{l_1}{2} j_1 \|Y_0\| \frac{l_2}{2} j_2 \langle A J A \| (a^+_{n_1 l_1 j_1} \tilde{a}_{n_2 l_2 j_2})^{(0)} \| A J A \rangle \]  

(B.2)

The radial functions of Eq. (B.2) are given as

\[ R_n(r) = \left[ \frac{2(2\nu)^{l_1+3/2} \Gamma(n+1)}{\Gamma(n+1+3/2)} \right]^{1/2} r^l e^{-\nu r^2} L_n^l(2\nu r^2) \]  

(B.3)

with \( \nu = \frac{m^2 \lambda \Omega}{2\hbar^2 c^2} \).

The reduced matrix element of the spherical harmonics from Eq. (B.1) is given by

\[ \langle l_1 \frac{1}{2} j_1 \|Y_K\| l_2 \frac{1}{2} j_2 \rangle = \frac{1}{\sqrt{4\pi}} \hat{j}_1 \hat{j}_2 \hat{l}_1 \hat{l}_2 (-1)^{l_1+\frac{1}{2}} \langle l_1 0 l_2 0 | K 0 \rangle \{ \begin{array}{ccc} j_1 & j_2 & K \\ l_2 & l_1 & \frac{1}{2} \end{array} \} \]  

(B.4)

For K = 0 this gives

\[ \langle l_1 \frac{1}{2} j_1 \|Y_0\| l_2 \frac{1}{2} j_2 \rangle = \frac{1}{\sqrt{4\pi}} \hat{j}_1 \hat{j}_2 \hat{l}_1 \hat{l}_2 (-1)^{l_1+\frac{1}{2}} \langle l_1 0 l_2 0 | 0 0 \rangle \{ \begin{array}{ccc} j_1 & j_2 & 0 \\ l_2 & l_1 & \frac{1}{2} \end{array} \} \]  

(B.5)

The Clebsch-Gordan coefficient reduces in the following way:

\[ \langle l_1 0 l_2 0 | 0 0 \rangle = (-1)^{l_1-0} \frac{1}{\sqrt{2l_2+1}} \langle l_1 0 0 0 | l_2 0 \rangle \]
leading to \( l_1 = l_2 \). For the 6j coefficient one obtains

\[
\begin{align*}
\begin{bmatrix} j_1 & j_2 & 0 \\ l & l & \frac{1}{2} \end{bmatrix} &= \begin{bmatrix} j_1 & l & \frac{1}{2} \\ l & j_2 & 0 \end{bmatrix} = \delta_{j_1 j_2} (-1)^{j_1 + l + \frac{1}{2}} \frac{1}{\sqrt{(2j_1 + 1)(2l + 1)}} \\
&= (-1)^{j + l + \frac{1}{2}} \frac{1}{\sqrt{(2j + 1)(2l + 1)}};
\end{align*}
\]

(B.7)

leading to \( j_1 = j_2 = j \). The term \( \Delta_{j l}^{1/2} \) refers to the triangulation of the three terms \( j, l, \) and \( \frac{1}{2} \), i.e. \(|j - l| \leq \frac{1}{2} \leq j + l\).

Taking everything together gives the explicit form of the zeroth order reduced matrix element for the spherical harmonic,

\[
\begin{align*}
\langle l_1 \frac{1}{2} j || Y_0 || l_1 \frac{1}{2} j \rangle &= \frac{1}{\sqrt{4\pi}} (2j + 1)(2l + 1)(-1)^{j + \frac{1}{2}} (-1)^l \frac{1}{\sqrt{2l + 1}} (-1)^{j + l + \frac{1}{2}} \frac{1}{\sqrt{(2j + 1)(2l + 1)}} \\
&= \frac{1}{\sqrt{4\pi}} \sqrt{2j + 1} (-1)^{j + l + l + \frac{1}{2}} \Delta_{j l}^{1/2} \\
&= \frac{1}{\sqrt{4\pi}} \sqrt{2j + 1} (-1)^{2j + 2l + 1} \Delta_{j l}^{1/2} \\
&= \frac{1}{\sqrt{4\pi}} \sqrt{2j + 1} \Delta_{j l}^{1/2}.
\end{align*}
\]

(B.8)

Here the term \((-1)^{2j + 2l + 1}\) was simplified to 1 since \(2j + 1\) is an even integer and as is \(2l\).

The next term to consider is \((-1) \times \langle AJ\lambda || (a_{n1j}^+ \bar{a}_{nlj})^{(0)} || AJ\lambda \rangle\), the reduced matrix elements in Eq. (B.1), absorbing a negative sign. However, since these values are read in we can leave the expression as is. The term \(\frac{1}{\sqrt{2K + 1}}\) evaluates to 1 when \(K = 0\).

Using the information from the different evaluation of the terms above, we obtain for the \( K = 0 \) multi-pole of the diagonal one-body density

\[
\rho_{sj}^{(0)} = \sum R_{n1l}(r) R_{n2j}(r) \left< l_{1/2} j || Y_0 || l_{1/2} j \right> \frac{1}{\sqrt{2l + 1}} \left< AJ\lambda || (a_{n1j}^+ \bar{a}_{nlj})^{(0)} || AJ\lambda \right> \\
= \sum R_{n1l}(r) R_{n2j}(r) \left< l_{1/2} j || Y_0 || l_{1/2} j \right> (-1) \left< AJ\lambda || (a_{n1j}^+ \bar{a}_{nlj})^{(0)} || AJ\lambda \right>.
\]
For the states with \(\rho\) needed. The only two terms that differ are the spherical component and the term \(\hat{a}_{nlj}^\dagger\), \(\hat{a}_{nlj}\) of the local density function.

\[
\begin{align*}
&= \sum \left[ \frac{2(2\nu)^{l+3/2}\Gamma(n_1 + 1)}{\Gamma(n_1 + l + \frac{3}{2})} \right]^{\frac{1}{2}} r^{2l} e^{-2\nu r^2} L_{n_1}^{l+\frac{1}{2}}(2\nu r^2) \Gamma(n_2 + l + \frac{3}{2})^{\frac{1}{2}} \times \frac{1}{\sqrt{4\pi}} \sqrt{2j + 1} \Delta_{jl}(2\nu r^2) \left\langle (a_{n_1l}^\dagger\tilde{a}_{nlj})^{(0)} | AJ\lambda \right\rangle \\
&= \sum \left[ \frac{2(2\nu)^{l+3/2}\Gamma(n_1 + 1)}{\Gamma(n_1 + l + \frac{3}{2})} \right]^{\frac{1}{2}} r^{2l} e^{-2\nu r^2} L_{n_1}^{l+\frac{1}{2}}(2\nu r^2) \Gamma(n_2 + l + \frac{3}{2})^{\frac{1}{2}} \times \frac{1}{\sqrt{4\pi}} \sqrt{2j + 1} \Delta_{jl}(2\nu r^2) \left\langle (a_{n_1l}^\dagger\tilde{a}_{nlj})^{(0)} | AJ\lambda \right\rangle \\
&= \frac{1}{\sqrt{4\pi}} \frac{2j + 1}{\sqrt{2j + 1}} \Delta_{jl}(2\nu r^2) \left\langle (a_{n_1l}^\dagger\tilde{a}_{nlj})^{(0)} | AJ\lambda \right\rangle.
\end{align*}
\] (B.9)

This final expression, Eq. (B.9), is the explicit form of the \(K = 0\) multipole contribution for the space-fixed local density, \(\rho_{sf}^{(0)}(r)\).

From the following Sections, one can realize that when calculating the local density for a nucleus A with total angular momentum \(J = 0\), only the \(K = 0\) multipole contributes.

**B.2 Derivation of the K=1 Multipole Term**

In this Section the three terms for the \(K = 1\) multipole that differ from the \(K = 0\) derivation are evaluated. A complete expression for \(\rho_{sf}^{(1)}(r)\) is not given due to the length needed. The only two terms that differ are the spherical component and the term \(\frac{1}{\sqrt{2k+1}}\).

For the \(K = 1\) multipole, the spherical component, Eq. (B.4) of the local density function is given by

\[
\left\langle l_1 \frac{1}{2} l_1 \left| Y_{1l_2}^1 \right| \frac{1}{2} l_2 \right\rangle = \frac{1}{\sqrt{4\pi}} \sum_{j_1 j_2 l_2} \langle l_1 l_2 0 10 \rangle \left\{ \begin{array}{c} j_1 \ j_2 \ 1 \\ l_1 \ l_2 \ \frac{1}{2} \end{array} \right\}.
\] (B.10)

For the states with \(l_1 = l_2\) the Clebsch-Gordan coefficient for \(\langle l_1 l_2 0 10 \rangle\) is 0 since \(l_1 + l_2 + 1\) must be an even number to be non-zero. This means the only two possible scenarios that give you non-zero contributions: \(l_1 = l_2 + 1, l_2 = l_1 + 1\), and

\[
\langle l_1 0 l_2 0 1 0 \rangle = \sqrt{3}(-1)^{l_2} (-l_2^2 - l_2 + l_1^2 + l_1)
\]

\[
\times \frac{1}{(l_2 + l_1)(l_2 + l_1 + 1)(l_2 + l_1 + 2)(l_2 - l_1 + 1)!(l_2 + l_1 + 1)!}
\] (B.11)
Assume $l_2 = l_1 + 1$. Then the 6j-terms are given explicitly as,

\[
\begin{align*}
&\begin{cases} 
  l + \frac{1}{2} (l + 1) + \frac{1}{2} 1 \\
  l \\
\end{cases} \begin{cases} 
  l \\
  l + 1 \\
\end{cases} = 0 \\
&\begin{cases} 
  l - \frac{1}{2} (l + 1) + \frac{1}{2} 1 \\
  l \\
\end{cases} \begin{cases} 
  l \\
  l + 1 \\
\end{cases} = 0 \\
&\begin{cases} 
  l - \frac{1}{2} (l + 1) - \frac{1}{2} 1 \\
  l \\
\end{cases} \begin{cases} 
  l \\
  l + 1 \\
\end{cases} = 0 \\
&\begin{cases} 
  l + \frac{1}{2} (l + 1) - \frac{1}{2} 1 \\
  l \\
\end{cases} \begin{cases} 
  l \\
  l + 1 \\
\end{cases} = (-1)^{-2l} \frac{1}{\sqrt{(l+1)(2l+1)(2l+3)}} \\
\end{align*}
\] (B.12)

for $l \geq 0$.

The second term $\frac{1}{\sqrt{2K+1}}$ evaluates to $\frac{1}{\sqrt{3}}$ for $K = 1$. If the expression $\langle JMK0|JM \rangle$ in Eq. (3.10) is taken into consideration, then

\[
\langle JM10|JM \rangle = \frac{M \sqrt{2J + 1}}{\sqrt{(2J^3 + 3J^2 + J)}} .
\] (B.13)

with the requirement of $J \geq \frac{1}{2}$. This means $J = 0$ cannot contribute to the $K = 1$ multipole.

### B.3 Derivation of the K=2 Multipole Term

In this Section the three terms for the $K = 1$ multipole that differ from the $K = 0$ derivation are evaluated. A complete expression for $\rho_{sf}^{(1)}(r)$ is not given due to the length needed. The only two terms that differ are the spherical component and the term $\frac{1}{\sqrt{2K+1}}$. For the $K = 2$ multipole, the spherical component, Eq. (B.4) of the local density function is given by

\[
\begin{align*}
\left\langle l_1 \frac{1}{2} j_1 | Y_{2}| l_2 \frac{1}{2} j_2 \right\rangle = \frac{1}{\sqrt{4\pi}} & j_1 j_2 l_1 l_2 (-1)^{l_1 + \frac{1}{2}} \left\langle l_1 0 l_2 0 | 20 \right\rangle \left\{ \begin{array}{ccc}
  j_1 & j_2 & 2 \\
  l_1 & l_2 & \frac{1}{2} \\
\end{array} \right\} ,
\end{align*}
\] (B.14)

The Clebsch-Gordan coefficient for $\langle l_1 0 l_2 0 | 20 \rangle$ is 0 when $l_1 - l_2 = 1$. The sum $l_1 + l_2 + 2$ must be even in order to have a non-zero coefficient. Thus, the only allowed combinations
of \( l_1 \) and \( l_2 \) are

\[
\begin{align*}
l_1 &= l_2 \quad \text{(B.15)} \\
l_1 &= l_2 + 2 \quad \text{(B.16)} \\
l_2 &= l_1 + 2 \quad \text{(B.17)}
\end{align*}
\]

From here the 6j-coefficients limit the possibilities even more.

For \( l_2 = l_1 + 2 \), the possible 6j combinations are

\[
\begin{align*}
\begin{cases}
    l + 5/2 & l + 1/2 & 2 \\
    l + 2 & l & 1/2 \\
    l + 3/2 & l + 1/2 & 2 \\
    l + 2 & l & 1/2 \\
    l + 5/2 & l - 1/2 & 2 \\
    l + 2 & l & 1/2 \\
    l + 3/2 & l - 1/2 & 2 \\
    l + 2 & l & 1/2
\end{cases} = 0
\end{align*}
\]

 \begin{align*}
\begin{cases}
    l + 1/2 & l + 1/2 & 2 \\
    l & l & 1/2 \\
    l - 1/2 & l + 1/2 & 2 \\
    l & l & 1/2 \\
    l + 1/2 & l - 1/2 & 2 \\
    l & l & 1/2 \\
    l - 1/2 & l - 1/2 & 2 \\
    l & l & 1/2
\end{cases} = 0
\end{align*}
\]

Since \( l_1 = l_2 + 2 \) would have the same 6j values, we only have the possible combination of \( l_1 = l_2 = l \).

The 6j coefficients for \( l_1 = l_2 = l \) are

\[
\begin{align*}
\begin{cases}
    l + 1/2 & l + 1/2 & 2 \\
    l & l & 1/2 \\
    l - 1/2 & l + 1/2 & 2 \\
    l & l & 1/2 \\
    l + 1/2 & l - 1/2 & 2 \\
    l & l & 1/2 \\
    l - 1/2 & l - 1/2 & 2 \\
    l & l & 1/2
\end{cases} &= -\frac{\sqrt{2 + l}(1 + 2l)(1 - 2l)}{\sqrt{2}(1 + l)(1 + 2l)}
\end{align*}
\]

\[
\begin{align*}
\begin{cases}
    l + 1/2 & l + 1/2 & 2 \\
    l & l & 1/2 \\
    l - 1/2 & l + 1/2 & 2 \\
    l & l & 1/2 \\
    l + 1/2 & l - 1/2 & 2 \\
    l & l & 1/2 \\
    l - 1/2 & l - 1/2 & 2 \\
    l & l & 1/2
\end{cases} &= \frac{\sqrt{3}l}{\sqrt{(l + 1^2)(1 + 2l^2)}}
\end{align*}
\]

\[
\begin{align*}
\begin{cases}
    l + 1/2 & l + 1/2 & 2 \\
    l & l & 1/2 \\
    l - 1/2 & l + 1/2 & 2 \\
    l & l & 1/2 \\
    l + 1/2 & l - 1/2 & 2 \\
    l & l & 1/2 \\
    l - 1/2 & l - 1/2 & 2 \\
    l & l & 1/2
\end{cases} &= \frac{\sqrt{3}l}{\sqrt{(l + 1^2)(1 + 2l^2)}}
\end{align*}
\]

\[
\begin{align*}
\begin{cases}
    l + 1/2 & l + 1/2 & 2 \\
    l & l & 1/2 \\
    l - 1/2 & l + 1/2 & 2 \\
    l & l & 1/2 \\
    l + 1/2 & l - 1/2 & 2 \\
    l & l & 1/2 \\
    l - 1/2 & l - 1/2 & 2 \\
    l & l & 1/2
\end{cases} &= \frac{\sqrt{2 + l}(1 + 2l)}{\sqrt{2}(2l^2 + l)}
\end{align*}
\]
For the first three $6j$ coefficients, we have $l \geq 1$, while for the last $6j$ value $l \geq \frac{3}{2}$.

The expression for the only remaining Clebsch-Gordan coefficient is given by

$$\langle l00|20 \rangle = (-1)^{l+1} \frac{\sqrt{5}(l^2 + l)}{\sqrt{(-3l^2 - 5l^2 + 10l^3 + 20l^4 + 8l^5)}} \quad \text{(B.20)}$$

For the term $\frac{1}{\sqrt{2K+1}}$, $K = 2$ results in the factor $\frac{1}{\sqrt{3}}$. If the expression $\langle JMK0|JM \rangle$ in Eq. (3.10) is taken into consideration, then

$$\langle JM20|JM \rangle = \frac{-\sqrt{1 + 2J(J + J^2 - 3M^2)}}{\sqrt{(-3J^2 - 5J^2 + 10J^3 + 20J^4 + 8J^5)}} \quad \text{(B.21)}$$

with the requirement of $J \geq 1$. This means $J = 0$ cannot contribute to the $K = 2$. 
APPENDIX C: NUMERICAL CONSIDERATIONS

In this appendix the details of the numerical calculation are discussed and some numerical checks are examined to prove our accuracy. In Section C.1, the numerical accuracy of the radial wave function of the HO, Eq. (3.5), is shown through the orthogonality condition. In Section C.2, a description of the input given by Pieter Maris and James Vary for the OBDME’s is outlined. For Section C.3, a numerical comparison between the code developed for this thesis and a similar code by Steven Weppner is described. Section C.4 describes the convergence of the Fourier transforms.

C.1 Numerical Accuracy of the Radial Wave Function

The radial wave function for the HO, Eq. (3.5), as derived in Appendix A, obeys an orthogonality relation. This condition can be used check the output of the specific piece of the wave function. The orthogonality relation for $R_{nl}(r)$ ensures that when the product of two radial wave function pieces are integrated, the result is given by

$$\int R_{nl}(r) R_{ml}(r) r^2 dr = \delta_{n,m} \cdot$$  \hspace{1cm} (C.1)

Table (C.1) shows the numerical accuracy of computing Eq. (C.1).
Table C.1: Numerical computation of the orthogonality relation between two radial wave functions shown in Eq. (C.1).

<table>
<thead>
<tr>
<th>1</th>
<th>n</th>
<th>m</th>
<th>Integral</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>2</td>
<td>0.105569889788621E-15</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>3</td>
<td>0.618420528599025E-16</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>4</td>
<td>-0.487048240652605E-16</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>5</td>
<td>0.702980191055393E-15</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>4</td>
<td>-0.487048240652605E-16</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.999999999999999E+00</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>2</td>
<td>0.999999999999998E+00</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>3</td>
<td>0.999999999999998E+00</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>4</td>
<td>0.999999999999999E+00</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>3</td>
<td>0.999999999999999E+00</td>
</tr>
</tbody>
</table>

C.2 Description of Maris-Vary Input Files

The input files by Pieter Maris and James Vary contain the input to their NCSM calculation together with coefficients of the computed Slater determinants [30]. Since we reconstruct the local densities from the computed coefficients, input parameters describing the nucleus under consideration must be the same in our code. A complete list along with descriptions of relevant parameters is given below.

Variables read in:

- Number of Protons and Neutrons: Used to confirm the nucleus being calculated.
- $\hbar \Omega$ or the Harmonic Oscillator Energy Scale: Must be the same between both calculations.
• Nucleon Mass for both Protons and Neutrons: Must be the same in both calculations.

• All quantum numbers for initial and final states from \( N = 0 \) to \( N = N_{\text{max}} \)
  
  – \( n_a \): radial quantum number \( n \) for initial state
  
  – \( l_a \): orbital quantum number \( l \) for initial state
  
  – \( 2j_a = 2 \) times \( j \) value for initial state
  
  – \( n_b = n \) value for final state
  
  – \( l_b = l \) value for final state
  
  – \( 2j_b = 2 \) times \( j \) value for final state
  
  – \( \text{index} = \) Identifier for quantum states
  
  – \( K = \) value of the multipole
  
  – \( \text{cls} = \) Class number: 1 for proton, 2 for neutron

• Total angular momentum \( J \) value of the quantum state

• \( M \) value: Projection \( J_Z \) of the quantum state

• Number of basis states used for a given quantum state

• OBDMEs corresponding to the index identifier for the initial and final state quantum numbers

C.3 Comparison Between a Code by Steve Weppner and the Current Matt Burrows Code

Previous computations by Prof. Stephen Weppner with \(^4\text{He}\) for \( N_{\text{max}} = 2 \) gave a check for the beginning calculations completed with our code. This comparison was carried out with the same \( N_{\text{max}} = 2 \) data set and without the removal of the center-of-mass. The
results of this work’s code and S. Weppner’s are given in Table C.2 for the point-proton and point-neutron radii calculated using Eq. (4.27). This comparison provided evidence that our code was equivalent to S. Weppner’s computation.

Table C.2: The point-proton and point-neutron radii calculated using Eq. (4.27) in this work’s code and in S. Weppner’s code.

<table>
<thead>
<tr>
<th></th>
<th>Proton</th>
<th>Neutron</th>
</tr>
</thead>
<tbody>
<tr>
<td>code SPW</td>
<td>1.66694825661979 48</td>
<td>1.6636071726910 084</td>
</tr>
<tr>
<td>code MB</td>
<td>1.66694825661979 95</td>
<td>1.6636071726910 137</td>
</tr>
</tbody>
</table>

C.4 Convergence of the Fourier Transforms

In the computation of this work’s local densities, there are a number of important variables that determine the convergence of the Fourier transformations. This work’s computation starts from a completed local density from Eq. (3.10), performs a Fourier transform using Eq. (3.22), removes the center-of-mass contribution by Eq. (4.26), performs a Fourier transform back to position space, and then uses Eq. (4.27) to compute the point radii. For all integrations required in the process outlined, we perform a cubic hermitian interpolation from a set of grid points, at which we calculate $\rho_{sf}(r)$, to a set of integration points that are used in a Simpson integration. The Simpson integration scheme is used due to the oscillatory behavior of the integral in the Fourier transformation. The maximum values $r_{max}$ and $q_{max}$ of the integration dictate the integration interval. The difficulty of the Fourier transform arises from the removal of the center of mass which requires Gaussian behavior at the large q-values of $\rho(q)$. If the large q part of the momentum space density does not exhibit a Gaussian fall off behavior then the removal of
the center of mass will cause part of the function to level off or diverge. If this happens, the RMS radius will diverge.

An example of the type of fall off behavior we expect to see after our two Fourier transformations is provided in Figure C.1 and C.2. Figure C.1 shows the exponential tail of the ground state local density $\rho_{sf}^{(0)}(r)$ of $^6$He in coordinate space as a function of $r^2$, while Figure C.2 shows the exponential tail of the ground state local density $\rho_{sf}^{(0)}(q)$ in momentum space as a function of $q^2$. Figure C.3 shows the ground state local density $\rho_{ti}^{(0)}(r)$ of $^6$He in coordinate space after a Fourier transform from coordinate to momentum space, center of mass motion removal, and Fourier transform from momentum back to coordinate space. From Figure C.3, it is easy to see that past $r^2 = 20 \text{fm}^2$ that the expected behavior of the local density is lost and we have reached the limit of our numerical accuracy.

![Graph](image)

**Figure C.1**: Coordinate space representation of the one-body local density $\rho_{sf}^{(0)}(r)$, for $^6$He in the ground state as a function of $r^2$. 
Figure C.2: Momentum space representation of the one-body local density $\rho_{sf}^{(0)}(q) \times Y_0^0(\hat{q})$, for $^6\text{He}$ in the ground state after a single Fourier transform as a function of $q^2$.

Figure C.3: Coordinate space representation of the one-body local density $\rho_{ti}^{(0)}(r)$, for $^6\text{He}$ in the ground state after the removal of the c.m. and Fourier transform to coordinate space as a function of $r^2$. 
First, we checked the convergence of the Fourier transform as a function of the values of $r_{\text{max}}$ and $q_{\text{max}}$ while keeping the number of grid points and the number of Simpson integration points constant. Here grid points refer to the points at which the local density is explicitly evaluated. This test is shown in Table C.3. Here the number of grid points is 9,000 while the number of integration points is 15,000. For this test, we chose the ground state state of $^6$He since it requires the largest $q_{\text{max}}$. It turns out that it is, for this case, numerically very difficult to recover the Gaussian behavior for large $q$ values. As seen in Table C.3, the values of $r_{\text{max}}$ and $q_{\text{max}}$ have a significant effect on the overall convergence of the RMS radius. There is a limit, roughly $q_{\text{max}} = 12.0 \text{ fm}^{-1}$ and $r_{\text{max}} = 12.0 \text{ fm}$, where the RMS radius seems to no longer be heading to convergence indicating that the number of grid points needs to be even higher. However, we can say that our RMS radii are converged, for the proton RMS radius, to 3 significant figures at $q_{\text{max}} = 9, 10, \text{ or } 11 \text{ fm}^{-1}$ and $r_{\text{max}} = 9, 10, \text{ or } 11 \text{ fm}$. The neutron RMS radius is converged to 5 significant figures at $r_{\text{max}} = 10 \text{ fm}$, $q_{\text{max}} = 10 \text{ fm}^{-1}$ and 4 significant figures at $r_{\text{max}} = 9 \text{ fm}$, $q_{\text{max}} = 9 \text{ fm}^{-1}$. For the remaining tests we will use the value of $q_{\text{max}} = 10 \text{ fm}^{-1}$ and $r_{\text{max}} = 10 \text{ fm}$.

Next we check the number of grid points while keeping the value of $q_{\text{max}} = 10 \text{ fm}^{-1}$ and $r_{\text{max}} = 10 \text{ fm}$ constant and the number of integration points constant at 15,000. The results of this test are in Table C.4. It is apparent from the table that increasing the number of grid points provides better convergence of the RMS radius though our program can only handle a maximum of 9500 grid points due to memory allocation. Since we only can get convergence of 3 significant figures, for the proton RMS radius, from the tests of $q_{\text{max}}$ and $r_{\text{max}}$ then it is unnecessary to get more than 4 significant figure convergence in the RMS radius. However, the number of grid points required for 4 significant figure convergence at different $q_{\text{max}}$ and $r_{\text{max}}$ values changes. Table C.5 shows this phenomenon more clearly by holding $q_{\text{max}} = 11 \text{ fm}^{-1}$, $r_{\text{max}} = 11 \text{ fm}$, and the number of integration points at 15,000. When $q_{\text{max}} = 11 \text{ fm}^{-1}$ and $r_{\text{max}} = 11 \text{ fm}$ the number of grid points required to reach 4
significant figure convergence is never achieved even at 9,000 grid points while Table C.4 shows $r_{\text{max}} = 10 \text{ fm}$ and $q_{\text{max}} = 10 \text{ fm}^{-1}$ converges easily at 1,500 grid points.

We last checked the effect of the integration points upon the convergence of the RMS radius. For this test we kept $r_{\text{max}} = 10 \text{ fm}$, $q_{\text{max}} = 10 \text{ fm}^{-1}$, and the number of grid points constant at 2,500. Table C.6 shows the results of this test. From the table it is clear that increasing or decreasing the number of integration points has little to no effect on the convergence of the RMS radius.

In conclusion, the required values to achieve 3 significant figure convergence for the RMS radius for both the proton and neutron local densities is $r_{\text{max}} = 10 \text{ fm}$, $q_{\text{max}} = 10 \text{ fm}^{-1}$, 1500 grid points, and 4000 integration points. The grid points and integration points can be increased and still achieve the same accuracy but the $r_{\text{max}}$ and $q_{\text{max}}$ values should not be increased past 11 fm and fm$^{-1}$, respectively, or the local densities will begin to diverge. Also, if $q_{\text{max}} = 11 \text{ fm}^{-1}$ and $r_{\text{max}} = 11 \text{ fm}$ then the number of grid points should be increased to 9,000 and the number of integration points to at least 9,500.

Table C.3: The Proton and Neutron RMS radii calculated for the ground state of $^6\text{He}$ with 9,000 grid points and 15,000 integration points.

<table>
<thead>
<tr>
<th>$r_{\text{max}}$ [fm] &amp; $q_{\text{max}}$ [fm$^{-1}$]</th>
<th>Proton RMS Radius [fm]</th>
<th>Neutron RMS Radius [fm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>1.43365596</td>
<td>2.28802502</td>
</tr>
<tr>
<td>7</td>
<td>1.40648589</td>
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</tr>
<tr>
<td>8</td>
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</tr>
<tr>
<td>9</td>
<td>1.40225253</td>
<td>2.27216951</td>
</tr>
<tr>
<td>10</td>
<td>1.39992926</td>
<td>2.27174340</td>
</tr>
<tr>
<td>11</td>
<td>1.39918603</td>
<td>2.27172884</td>
</tr>
<tr>
<td>12</td>
<td>1.33313434</td>
<td>2.27172860</td>
</tr>
</tbody>
</table>
Table C.4: The Proton and Neutron RMS radii calculated for the ground state of $^6\text{He}$ with varying grid points, 15,000 integration points, $r_{\text{max}} = 10$ fm, and $q_{\text{max}} = 10$ fm$^{-1}$.

<table>
<thead>
<tr>
<th>Grid Points</th>
<th>Proton RMS Radius [fm]</th>
<th>Neutron RMS Radius [fm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>250</td>
<td>1.26588365</td>
<td>2.27174042</td>
</tr>
<tr>
<td>500</td>
<td>1.39893256</td>
<td>2.27174324</td>
</tr>
<tr>
<td>750</td>
<td>1.39986904</td>
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<td>1500</td>
<td>1.39992947</td>
<td>2.27174339</td>
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<tr>
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<td>2.27174340</td>
</tr>
<tr>
<td>5000</td>
<td>1.39993434</td>
<td>2.27174340</td>
</tr>
<tr>
<td>9000</td>
<td>1.39992926</td>
<td>2.27174340</td>
</tr>
</tbody>
</table>

Table C.5: The Proton and Neutron RMS radii calculated for the ground state of $^6\text{He}$ with varying grid points, 15,000 integration points, $r_{\text{max}} = 11$ fm, and $q_{\text{max}} = 11$ fm$^{-1}$.

<table>
<thead>
<tr>
<th>Grid Points</th>
<th>Proton RMS Radius [fm]</th>
<th>Neutron RMS Radius [fm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1500</td>
<td>1.40784202</td>
<td>2.27172883</td>
</tr>
<tr>
<td>2500</td>
<td>1.40118486</td>
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<tr>
<td>5000</td>
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<td>2.27172884</td>
</tr>
<tr>
<td>7500</td>
<td>1.40074731</td>
<td>2.27172884</td>
</tr>
<tr>
<td>9000</td>
<td>1.39918603</td>
<td>2.27172884</td>
</tr>
</tbody>
</table>
Table C.6: The Proton and Neutron RMS radii calculated for the ground state of $^6$He with 2,500 grid points, varying integration points, $r_{\text{max}} = 10$ fm, and $q_{\text{max}} = 10$ fm$^{-1}$.

<table>
<thead>
<tr>
<th>Integration Points</th>
<th>Proton RMS Radius [fm]</th>
<th>Neutron RMS Radius [fm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>4,000</td>
<td>1.39992992</td>
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</tr>
<tr>
<td>6,000</td>
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<td>2.27174340</td>
</tr>
<tr>
<td>9,000</td>
<td>1.39992968</td>
<td>2.27174340</td>
</tr>
<tr>
<td>12,000</td>
<td>1.39993063</td>
<td>2.27174340</td>
</tr>
<tr>
<td>15,000</td>
<td>1.39993237</td>
<td>2.27174340</td>
</tr>
</tbody>
</table>

Lastly, we wish to examine which region in the interval $r = 0$ to $r = 10$ fm is critically impacted by the number of grid points. To achieve this, we divide the interval into five sections, A ($r = 0$ fm to $r = 2$ fm), B ($r = 2$ fm to $r = 4$ fm), C ($r = 4$ fm to $r = 6$ fm), D ($r = 6$ fm to $r = 8$ fm), and E ($r = 8$ fm to $r = 10$ fm). Then we lower the number of grid points separately in each sub-interval from 800 to 50. The resulting momentum space densities are depicted in Fig. C.4 as a function of $q^2$. The biggest shift in the local density comes from decreasing the number of points in section A ($r = 0$ fm to $r = 2$ fm).

Decreasing points in section D and E ($r = 6$ fm to $r = 10$ fm) doesn’t seem to effect the Gaussian behavior at large $q$ values and thus will not contribute significantly to the final result no matter the number of points. From this figure, one can conclude that a large number of points is required in at least section A, a moderate to low amount of points are needed in section B and C, and D and E need a very low amount of points to achieve Gaussian behavior at large $q$ values.

Lastly, we study the size of the integrand at different values of $q$. The integral values of the Fourier transform for specific $q$ values of 1 fm$^{-1}$, 2 fm$^{-1}$, 3 fm$^{-1}$, 5 fm$^{-1}$, and 10 fm$^{-1}$ are given in Fig. C.5. It is apparent that for the $r$ values less then about $r = 4$ fm, the local density must be very well defined in order to eliminate the error from adding and
subtracting, relatively, large values. This means that sections A and B \((r = 0 \text{ fm to } r = 4 \text{ fm})\) contribute most to the error in the Fourier transform of the local density.

![Figure C.4: The momentum space one-body local density \(\rho_{s.f.}^{(0)}(q)\), for \(^6\text{He}\) in the ground state as a function of \(q^2\). Grid points between different subsections of the coordinate space local density are changed from 800 to 50.](image-url)
Figure C.5: Fourier transformation integral values for $4\pi \rho(r) r^2 j_0(qr)$ for five different values of $q$ as function of $r$. The values of $q$ are given in the legends.
**APPENDIX D: FLOWCHART**

This flow chart is the computational order of operations for computing the translationally invariant local density and rms radii. The blue nodes on the flow chart represent input, the yellow nodes represent subroutines, and the red nodes are the operations of the main program.
For each r value calculate
\[ \rho_{sf}^{(K)}(r) = R_{n_1} \times R_{n_2} \times \left\langle \left( \frac{1}{2} j_1 || Y_K || \frac{1}{2} j_2 \right) \times \frac{-1}{\sqrt{2K+1}} \times \left\langle AJ\lambda || (\alpha_{n_1}^l \alpha_{n_2}^l)^{(K)} \right\rangle AJ\lambda \right\rangle \]

Fourier transform \( \rho_{sf}^{(K)}(r) \) to \( \rho_{sf}^{(K)}(q) \)

Remove the center-of-mass contribution \( e^{-\frac{r^2q^2}{4\pi}} \) from \( \rho_{sf}^{(0)}(q) \)

Fourier Transform back to \( \rho_{sf}^{(K)}(r) \) from \( \rho_{sf}^{(K)}(q) \)

Calculate the RMS radius by
\[ \langle r^2 \rangle^{1/2} = \left[ \frac{\int \rho_{sf}(r) r^2 dr}{\int \rho_{sf}(r) dr} \right]^{1/2} \]