Removing center of mass effects in response function and sum rule calculations based on the harmonic oscillator basis

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Response functions are at the heart of any comparison of theory with experiment in studies of the nuclear dynamics with electroweak probes. Calculations performed in the laboratory frame often suffer from center of mass contaminations that need to be removed. By confining the system in a harmonic oscillator, we derive a set of analytical formulas to subtract the center of mass effects from calculations of response functions and associated sum rules. After a general analytical derivation, we first deal specifically with the longitudinal response function appearing in electron scattering and provide expressions for the center of mass correcting functions. Next, we present a proof of principle study for the case of the electric dipole sum rules in a two-body problem with a numerical implementation of our formalism. These steps pave the way to applying the proposed method to heavier nuclei in the future.

I. INTRODUCTION

The nucleus is a self bound system, made by many interacting protons and neutrons. In contrast to an atomic system, when solving the nucleus as a quantum many-body problem one does not have an external potential that provides confinement nor a natural center for the coordinate system. Hence, one typically refers the A-nucleons coordinates \( \{ r_k \} \) to an arbitrarily fixed coordinate center. One possible choice for the coordinate center is the laboratory frame, another possible choice is the center of mass (CoM) frame, also called internal or intrinsic frame. After defining the CoM coordinate for \( A \) equal-mass particles as

\[
\mathbf{R}_{\text{CoM}} = \frac{1}{A} \sum_k r_k ,
\]

one may, in fact, introduce the internal coordinates

\[
r_k' = r_k - \mathbf{R}_{\text{CoM}},
\]

where one essentially takes the CoM as the reference center of the coordinate system.

In terms of the single-particle coordinates \( \{ r_k \} \), the nuclear Hamiltonian is the sum of the kinetic and potential energy

\[
\hat{\mathcal{H}} = \hat{T} + \hat{V} = \sum_k \frac{p_k^2}{2m_N} + \sum_{k<j} \hat{V}(r_k - r_j),
\]

where \( m_N \) denotes the nucleon mass, an average of the proton and neutron masses, and where only two-body forces are considered without writing explicitly their spin-isospin dependence\(^1\). The potential \( \hat{V} \) in Eq. (3) depends only on the difference of the particle-coordinates and is thus translational invariant, namely it is the same independently on the center of the reference frame.

The Hamiltonian (3) can be written as

\[
\hat{\mathcal{H}} = \hat{T}^I + \hat{T}_{\text{CoM}}^I ,
\]

where \( \hat{T}_{\text{CoM}}^I = \frac{p_{\text{CoM}}^2}{2m_N} \) is the CoM kinetic energy and \( \hat{T}^I \) is the internal (I) Hamiltonian

\[
\hat{T}^I = \sum_k \frac{\mathbf{p}_k^2}{2m_N} + \sum_{k<j} \hat{V}(r_k - r_j) = \sum_k \frac{\mathbf{p}_k'^2}{2m_N} + \sum_{k<j} \hat{V}(r_k' - r_j') ,
\]

where \( \mathbf{p}_k' \) are the momenta relative to the CoM momentum. It is to note that \( \hat{T}^I \) is translational invariant, namely it has the exact same form, e.g., in terms of particle-coordinates \( \{ r_k \} \) referred to the laboratory frame or in term of the internal coordinate \( \{ r_k' \} \) referred to the CoM.

Because relative coordinates (2) are not linearly independent, it is customary to transform the \( A \)-particles coordinate system \( \{ r_k \} \) into a system where coordinates are made by \( \mathbf{R}_{\text{CoM}} \) and \( \{ A - 1 \} \) linearly independent relative position vectors, called the Jacobi coordinates [1]. The latter can be used to describe the internal dynamics of \( \hat{T}^I \). Working with Jacobi coordinates and dealing only with \( \hat{T}^I \), disregarding completely the CoM, is the preferred choice when studying light nuclei (see, e.g., Refs. [2, 3]). Solving for \( \hat{T}^I \) is indeed the only interesting part in the description of nuclear properties. However, the antisymmetrization of the wave function is typically the limiting factor in extending this approach to nuclei with \( A > 7 \) [4, 5]. To study medium to heavy nuclei, the typical choice is that of the single-particle coordinates \( \{ r_k \} \), because antisymmetrization is easily obtained with

\(^1\) Note that adding three-body forces does not change the presented formalism.
Slater determinants defined in terms of single-particle states [6].

Clearly, whenever the Hamiltonian can be written as the sum of an intrinsic and a CoM component as in Eq. (4), its eigenstates can be factorized into a product of the CoM wave function and the internal wave function

$$|\Psi\rangle = |\Psi^I\rangle \otimes |\Psi^\text{CoM}\rangle$$

(6)

with the corresponding energy given by the sum of the two subsystem energies $E^I = \epsilon + E$. Here, we use the Greek letter for the internal energy and the Latin letter for the CoM energy. If the Hamiltonian can be written as in Eq. (4), the separation of the CoM component from the internal part is ensured by (6), so that knowing $|\Psi^\text{CoM}\rangle$ one can extract the internal wave functions, even when working with a non-translational invariant Hamiltonian. Whether the factorization in Eq. (6) is preserved or not, depends on the method used to represent the nuclear wave function and to solve the Hamiltonian problem.

One way to solve the Schrödinger equation for the nuclear Hamiltonian is to expand the wave function on a complete set of basis states. After truncation of that basis, one turns to the task of diagonalizing the Hamiltonian matrix on the basis of choice. The favorite basis in nuclear physics is the harmonic oscillator basis, the traditional application being the nuclear shell model [7].

With the harmonic oscillator basis defined in terms of single-particle coordinates $\{r_k\}$, the exact factorization of Eq. (6) is preserved only when one uses the harmonic oscillator in a complete $N\hbar\Omega$ space [8], where $N$ is the harmonic oscillator quantum number and $\hbar\Omega$ the harmonic oscillator frequency. When the basis is truncated in any other way, the factorization may not hold. This causes the appearance of ”spurious CoM states” which contaminate the theoretical description of the internal dynamics. This problem, also known as ”CoM problem”, has been discussed in the literature very early in the history of nuclear many-body theory [8–11], but also more recently, where various solutions have been proposed (mostly for ground-state properties) for no-core shell model [12] or coupled-cluster theory calculations [13, 14].

In this paper, we want to analyze the case of response functions and related sum rules, which involve the excitation of the nucleus. Recently, it was shown that the Lawson method [10] can be numerically implemented to treat the CoM spurious states in sum rule calculations [15].

Here, we want instead to present an analytical method to remove center of mass effects in the case of response function calculated in single particle basis. The method is valid for any such basis, as long as the ground state and response functions are calculated with high enough accuracy. Nevertheless, we expect it to work best for the harmonic oscillator basis.

When working with the harmonic oscillator basis, one typically adds a CoM potential $V^\text{CoM} = \frac{1}{2} A m_N \Omega \mathbf{R}^2$, to $\hat{H}$, so that the new Hamiltonian becomes

$$\hat{H} = \hat{H}^I + \hat{H}^\text{CoM},$$

(7)

with $\hat{H}^\text{CoM} = \hat{T}^\text{CoM} + \hat{V}^\text{CoM}$. This Hamiltonian obviously admits the factorization of Eq. (6) and the CoM wave functions $|\Psi^\text{CoM}\rangle$ are known harmonic oscillator eigenstates.

In the following, we will assume that $\hat{H}$ has already been solved in the coordinates $\{r_k\}$, which we call the laboratory frame, and we will derive an analytical connection to calculations in the internal frame governed by $\hat{H}^I$. Our goal is to derive such connections for response functions and sum rules that are induced by external operators which can be written in the following form

$$\hat{\mathcal{O}} = \hat{\mathcal{O}}^I \hat{\mathcal{O}}^\text{CoM},$$

(8)

with $\hat{\mathcal{O}}^I$ acting only on the internal wave function, and $\hat{\mathcal{O}}^\text{CoM}$ on the CoM one. Most of the operators used in electroweak processes have this form [16, 17] and we will show later that our formalism can be generalized also to the case where $\hat{\mathcal{O}} = \hat{\mathcal{O}}^I + \hat{\mathcal{O}}^\text{CoM}$, which include another large category of electroweak operators.

The paper is structured as follows. In Section II and Section III we present the analytical derivation of our method for response functions and related sum rules, respectively. In Section IV we present first the example of the electron scattering process, while in Section V we deal with the photoabsorption case as a second example, where we provide a numerical implementation of our analytical formulae. Finally, in Section VI we draw our conclusions.

II. THE RESPONSE FUNCTION

The response function is the basic quantity that describes the interaction of a nuclear system with external probes and is defined as [18]

$$R(\omega) = \sum_{F,0} \left| \langle \Psi_F | \hat{\mathcal{O}} | \Psi_0 \rangle \right|^2 \delta (E_F - E_0 - \hbar\omega).$$

(9)

Here, $\omega$ is the energy transfer, $\Psi_0$ and $\Psi_F$ are the initial (ground state) and final state wave functions with energy $E_{0/F}$, respectively, while $\hat{\mathcal{O}}$ is the excitation operator, determined by the probe. The summation symbol in Eq. (9) has to be understood as a sum on all discrete and an integral on all the continuous quantum numbers in the final state, cumulatively denoted by $F$. An average on the initial state quantum numbers is also typically included in the definition and is denoted here with $\bar{0}$. Finally, the delta function ensures the conservation of the energy.

Let us assume that we have already solved this problem in the laboratory frame working with coordinates $\{r_k\}$. Our goal is to derive a formalism to separate the total response function of Eq. (9) calculated in the laboratory
frame into a center of mass term —to be removed—and the intrinsic response function, that pertains to the degrees of freedom included in $\hat{H}^I$ and $\hat{O}^I$. The latter is what one would directly obtain working in the center of mass frame, e.g., using Jacobi coordinates [19–23]. Because

$$[\hat{H}^I, \hat{H}^{\text{CoM}}] = 0, \quad (10)$$

we can take the eigenstates of $\hat{H}^I$, which we call $|\Psi_{ejm}\rangle$, and those of $\hat{H}^{\text{CoM}}$, which we call $|\Psi_{EJM}^{\text{CoM}}\rangle$, and choose the coupled outer product [24]

$$|\Psi_{EJM}\rangle = \left[|\Psi_{ejm}\rangle \otimes |\Psi_{EJM}^{\text{CoM}}\rangle\right]_{J}^{M}, \quad (11)$$

as basis for $\hat{H}$. This basis simultaneously diagonalizes $\hat{H}^I$, $\hat{H}^{\text{CoM}}$ and $\hat{H}$ and constitutes a set of states with good angular momentum quantum numbers $j$ (intrinsic), $J$ (CoM) and $J$ (total) with angular momentum projection $m$ (intrinsic), $M$ (CoM) and $M$ (total).

For the initial CoM state we have $J_0 = M_0 = 0$ so that the initial state becomes

$$|\Psi_0\rangle \rightarrow |\Psi_{E_0,J_0,M_0}\rangle = |\Psi_{e_0,j_0,m_0}^{\text{CoM}}\rangle |\Psi_{E_0,00}\rangle, \quad (12)$$

with $E_0 = \varepsilon_0 + E_0$. For the final state, in Eq. (11) we write the coupling explicitly using Clebsch-Gordan coefficients [24], so that the final state in our basis becomes

$$|\Psi_F\rangle \rightarrow |\Psi_{EJM}\rangle = |\Psi_{E(j)JM}\rangle = \sum_{mJ} \langle jmJ |JM|\Psi_{ejm}\rangle |\Psi_{EJM}^{\text{CoM}}\rangle \quad (13)$$

with $E = \varepsilon + E$. We note that due to rotational invariance the energies do not depend on the angular momentum projection.

In order to calculate the response function of Eq. (9) we need to consider the transition amplitude $\langle \Psi_{EJM}|\hat{O}|\Psi_{E_0,J_0,M_0}\rangle$ from an initial state $|\Psi_{E_0,J_0,M_0}\rangle$ to a final state $|\Psi_{EJM}\rangle$, take the square of it and perform a sum over all possible final states and average on the initial state quantum numbers. In our notation, the total response function of Eq. (9) becomes

$$R(\omega) = \frac{1}{2J_0 + 1} \sum_{\varepsilon} \sum_{JM} \left|\langle \Psi_{EJM}|\hat{O}|\Psi_{E_0,J_0,M_0}\rangle\right|^2 \delta(E - E_0 - \hbar\omega), \quad (14)$$

where we note that the $\sum_{J,j,J}$ are not free sums, but are connected to each other by angular momentum coupling rules. The summation $\sum_{\varepsilon}$ has to be intended as the sum of any quantum number the energy may depend on, but the angular momentum.

Using Eqs. (12) and (13), the squared matrix element in Eq. (14) becomes

$$\sum_{JM} \sum_{jM} \left|\langle \Psi_{E(j)JM}|\hat{O}|\Psi_{E_0,J_0,M_0}\rangle\right|^2 = \sum_{JM} \sum_{jM} \sum_{\varepsilon} \sum_{jmJM} \left|\langle jmJM|\Psi_{ejm}\rangle |\Psi_{EJM}^{\text{CoM}}\rangle\right|^2 \sum_{JM} \sum_{jM} \sum_{\varepsilon} \sum_{jmJM} \left|\langle jmJM|\Psi_{ejm}\rangle |\Psi_{EJM}^{\text{CoM}}\rangle\right|^2 \delta(E - E_0) \delta\left(E - E_0 - \hbar\omega\right) \quad (15)$$

Finally, using the factorization ansatz of Eq. (8), we obtain the following expression for the response function

$$R(\omega) = \frac{1}{2J_0 + 1} \sum_{\varepsilon} \sum_{jmJM} \left|\langle ejm|\hat{O}|1\rangle |\Psi_{e_0,j_0,m_0}^{\text{CoM}}\rangle\right|^2 \sum_{JM} \sum_{jM} \left|\langle \Psi_{EJM}^{\text{CoM}}|\hat{O}|\Psi_{E_0,00}\rangle\right|^2 \delta(E - E_0 - \hbar\omega) \quad (17)$$

It is to note that due to the presence of the delta function that depends on both the intrinsic and the CoM energies, we can not use completeness and perform the sum over the CoM quantum numbers $J, M$.

Next, one realizes that given $\hat{O}^{\text{CoM}}$ it is possible to calculate the CoM matrix elements $\langle \Psi_{EJM}^{\text{CoM}}|\hat{O}|\Psi_{E_0,00}\rangle$. Indeed, they can even be calculated analytically most of the time, since the CoM wave functions are harmonic oscillator states. Furthermore, one can rewrite the delta function as

$$\delta(E - E_0 - \hbar\omega) = \delta(\omega = E - E_0 + \varepsilon_0 - \varepsilon_0 - \hbar\omega)$$

and because the CoM is in a harmonic oscillator state, excitation energies will be quantized so as to satisfy

$$E - E_0 = N\hbar\Omega, \quad N = 0, 1, 2, \ldots, \quad (18)$$

with $N = 2N_r + J$, where $N_r$ is the radial quantum number and $J \leq N$. This allows one to rewrite Eq. (17) as

$$R(\omega) = \frac{1}{2J_0 + 1} \sum_{\varepsilon} \sum_{jmJM} \left|\langle ejm|\hat{O}|1\rangle |\Psi_{e_0,j_0,m_0}^{\text{CoM}}\rangle\right|^2 \times \sum_{JM} \left|\langle \Psi_{EJM}^{\text{CoM}}|\hat{O}|\Psi_{E_0,00}\rangle\right|^2 \delta(\varepsilon - \varepsilon_0 - N\hbar\Omega - \hbar\omega) \quad (19)$$

where $\sum_{\varepsilon}$ has been split into a sum on the internal energy $\Sigma_\varepsilon$ and a sum on the CoM energy. Because the latter
only depends on the quantum number $N$, the sum on the energy becomes $\sum_{N}$ and the label $E$ in the wave function can be substituted just with $N$ as $|\Psi_{EJM}^{\text{CoM}}\rangle \rightarrow |\Psi_{NJM}^{\text{CoM}}\rangle$, with $N = 0$ for the ground state.

Next, we define the CoM transition probabilities as

$$K_N^{\text{CoM}} = \sum_{J \leq N} \sum_{M=-J}^{+J} \left| \langle \Psi_{NJM}^{\text{CoM}} | \hat{O} | \Psi_{0JM}^{\text{CoM}} \rangle \right|^2,$$

which must fulfill the relation

$$\sum_{N=0}^{\infty} K_N^{\text{CoM}} = \langle \Psi_0^{\text{CoM}} | \hat{O} | \Psi_0^{\text{CoM}} \rangle,$$

as the sum of the transition probabilities to all excited states must always be equal to 1.

Finally, the total response function (17) can be written as

$$R(\omega) = \frac{1}{2\hbar \omega} + \sum_{m_{0J} \neq m} \left| \langle \Psi_{\epsilon_{\text{ejm}}^{\text{CoM}}} | \hat{O} | \Psi_{\epsilon_{\text{ejm}_{0J}}^{\text{CoM}}} \rangle \right|^2 \sum_{N} K_N^{\text{CoM}} \delta (\epsilon - \epsilon_0 + \hbar \Omega - \hbar \omega).$$

At this point, it is useful to introduce the intrinsic response function,

$$R^I(\omega - N\Omega) = \frac{1}{2\hbar \omega} + \sum_{m_{0J} \neq m} \left| \langle \Psi_{\epsilon_{\text{ejm}}^{\text{CoM}}} | \hat{O} | \Psi_{\epsilon_{\text{ejm}_{0J}}^{\text{CoM}}} \rangle \right|^2 \delta (\epsilon - \epsilon_0 + \hbar \Omega - \hbar \omega).$$

If the energy transfer is smaller than the energy of level $N$, then the system cannot be excited to that energy level. Mathematically, we demand therefore that $\omega - N\Omega \geq 0$. Finally, we can connect the total response function with the intrinsic response function and write the following system of equations

$$R(\omega) = \sum_{N} K_N^{\text{CoM}} R^I(\omega - N\Omega), \quad \omega - N\Omega \geq 0.$$  \hspace{1cm} (25)

The idea of this formalism is actually to draw $R^I(\omega)$ for a known calculation or $R(\omega)$ at any value of $\omega$ in a certain range of interest. As a consequence of the condition in Eq. (25), if $\omega < \Omega$ then $N$ must be zero and Eq. (25) is reduced to $R(\omega) = K_0^{\text{CoM}} R^I(\omega)$. At higher energy transfer, $\Omega < \omega < 2\Omega$, the possible energy levels will include $N = 1$ and so on. Thus, we can write

$$0 \leq \omega < \Omega \rightarrow N = 0 : \quad R(\omega) = K_0^{\text{CoM}} R^I(\omega),$$

$$\Omega \leq \omega < 2\Omega \rightarrow N = 1 : \quad R(\omega) = K_0^{\text{CoM}} R^I(\omega) + K_1^{\text{CoM}} R^I(\omega - \Omega),$$

$$2\Omega \leq \omega < 3\Omega \rightarrow N = 2 : \quad R(\omega) = K_0^{\text{CoM}} R^I(\omega) + K_1^{\text{CoM}} R^I(\omega - \Omega) + K_2^{\text{CoM}} R^I(\omega - 2\Omega),$$

$$\vdots$$

$$N\Omega \leq \omega < (N + 1)\Omega : \quad R(\omega) = K_0^{\text{CoM}} R^I(\omega) + \sum_{m=1}^{N} K_m^{\text{CoM}} R^I(\omega - m\Omega).$$

In the first line of Eq. (26) we have only one unknown, namely $R^I(\omega)$. Both $R^I(\omega)$ and $R^I(\omega - \Omega)$ in the second line are unknown, but we can calculate the latter using the first line. Indeed, this quantity depends on an energy in the region $\omega < \Omega$, that we can calculate with the first line of Eq. (26). After this is done we can solve the second line. We then solve the third line with the help of the first and second line, and so on. For a given energy range $N\Omega \leq \omega < (N + 1)\Omega$, the recursion can be written as

$$R^I(\omega) = \frac{1}{K_0^{\text{CoM}}} \left[ R(\omega) - \sum_{m=1}^{N} K_m^{\text{CoM}} R^I(\omega - m\Omega) \right].$$

This is the first important recursive equation resulting from our formalism. In essence, following this procedure for each region of $\omega$ we can find the response function $R^I(\omega)$ as calculated in the intrinsic frame from a calculation of $R(\omega)$ in the laboratory frame, given that we have calculated the CoM transition probabilities of Eq. (20).
III. SUM RULES

In this section we apply our formalism to other important quantities in scattering processes, namely the sum rules. The latter are defined as integrals of the response function

$$S_n = \int_0^\infty d\omega \omega^n R(\omega),$$

(28)

where \( n \) is typically an integer number. Sum rules are sometimes easier to calculate than the response function itself, see, e.g., Refs. [15, 26, 27]. Let us assume that a generic sum rule of the total system is calculated in the laboratory frame and use again the known \( K_{N\text{CoM}} \) to extract only the intrinsic part, which we are interested in.

If we multiply the relation of Eq. (27) by \( \omega^n \) and take an integral from zero to infinity, we will obtain a relation for the sum rules. Recalling that \( K_{N\text{CoM}} \) does not depend on \( \omega \) and that a response for negative energies is zero, we can write

$$S_n = \int_0^\infty d\omega \omega^n R(\omega) = K_{0\text{CoM}} \int_0^\infty d\omega \omega^n R^I(\omega) + K_{1\text{CoM}} \int_0^\infty d\omega \omega^n R^I(\omega - \Omega) + K_{2\text{CoM}} \int_{2\Omega}^\infty d\omega \omega^n R^I(\omega - 2\Omega) + \ldots.$$  

(29)

Introducing the intrinsic sum rule

$$S_n^I = \int_0^\infty d\omega \omega^n R^I(\omega)$$

(30)

and redefining the integration variable in each integral

$$\omega - \Omega = \omega_1 \quad \rightarrow \quad \omega = \omega_1 + \Omega$$  

(31)

$$\omega - 2\Omega = \omega_2 \quad \rightarrow \quad \omega = \omega_2 + 2\Omega$$

$$\vdots$$

$$\omega - m\Omega = \omega_m \quad \rightarrow \quad \omega = \omega_m + m\Omega$$

we obtain

$$S_n = K_{0\text{CoM}} S_n^I + K_{1\text{CoM}} \int_0^\infty d\omega_1 R^I(\omega_1) (\omega_1 + \Omega)^n + K_{2\text{CoM}} \int_0^\infty d\omega_2 R^I(\omega_2) (2\Omega)^n + \ldots$$

(32)

$$+ K_{m\text{CoM}} \int_0^\infty d\omega_m R^I(\omega_m) (m\Omega)^n + \ldots.$$  

The binomial coefficients \((x + y)^n = \sum_{k=0}^{n} \binom{n}{k} x^{n-k} y^k\) can be used to rewrite

$$(m\Omega + \omega_m)^n = \sum_{k=0}^{n} \binom{n}{k} (m\Omega)^{n-k} \omega_m^k$$

(33)

and obtain

$$S_n = K_{0\text{CoM}} S_n^I + K_{1\text{CoM}} \sum_{k=0}^{n} \binom{n}{k} (\Omega)^{n-k} \omega_1^k + K_{2\text{CoM}} \sum_{k=0}^{n} \binom{n}{k} (2\Omega)^{n-k} \omega_2^k + \ldots$$

(34)

$$+ K_{m\text{CoM}} \sum_{k=0}^{n} \binom{n}{k} (m\Omega)^{n-k} \omega_m^k + \ldots.$$  

Since the \( \omega_m \) are dummy integration variables, we can at this point replace them by \( \omega \), so that the integrals become sum rules and we obtain

$$S_n = K_{0\text{CoM}} S_n^I + K_{1\text{CoM}} \sum_{k=0}^{n} \binom{n}{k} (\Omega)^{n-k} \int_0^\infty d\omega R^I(\omega) \omega^k + K_{2\text{CoM}} \sum_{k=0}^{n} \binom{n}{k} (2\Omega)^{n-k} \int_0^\infty d\omega R^I(\omega) \omega^k + \ldots$$

(35)

$$+ K_{m\text{CoM}} \sum_{k=0}^{n} \binom{n}{k} (m\Omega)^{n-k} \int_0^\infty d\omega R^I(\omega) \omega^k + \ldots.$$  

$$= K_{0\text{CoM}} S_n^I + K_{1\text{CoM}} \sum_{k=0}^{n} \binom{n}{k} (\Omega)^{n-k} S_k^I + K_{2\text{CoM}} \sum_{k=0}^{n} \binom{n}{k} (2\Omega)^{n-k} S_k^I + \ldots$$

$$+ K_{m\text{CoM}} \sum_{k=0}^{n} \binom{n}{k} (m\Omega)^{n-k} S_k^I + \ldots.$$  

$$= K_{0\text{CoM}} S_n^I + \sum_{k=0}^{n} \binom{n}{k} (\Omega)^{n-k} S_k^I [K_{1\text{CoM}} + K_{2\text{CoM}} 2^{n-k} + \ldots + K_{m\text{CoM}} m^{n-k} + \ldots].$$
Thus, we can write the following recursive relation for the intrinsic sum rules

\[ S_n = K_0^{\text{CoM}} S_n^I + \sum_{k=0}^{n} \binom{n}{k}(\Omega)^{n-k} S_k^I \sum_{m=1}^{\infty} K_m^{\text{CoM}} m^{-n-k}. \]  

(36)

To obtain intrinsic sum rules from a calculation in the laboratory frame, we clearly have an iterative procedure. First, we find the intrinsic sum rule of order zero \( S_0^I \) as

\[ S_0^I = \frac{S_0}{\sum_{m=0}^{\infty} K_m^{\text{CoM}}}. \]  

(37)

Second, to obtain the intrinsic sum rule of order one we use

\[ S_1^I = K_0^{\text{CoM}} S_1^I + \sum_{k=0}^{1} \binom{1}{k}(\Omega)^{1-k} S_k^I \sum_{m=1}^{\infty} K_m^{\text{CoM}} m^{-1-k} \]  

(38)

\[ = S_1^I \sum_{m=0}^{\infty} K_m^{\text{CoM}} + \Omega S_0^I \sum_{m=1}^{\infty} m K_m^{\text{CoM}}, \]

so that the intrinsic sum rule can be obtained as

\[ S_1^I = \frac{1}{\sum_{m=0}^{\infty} K_m^{\text{CoM}} \left[ S_1 - \Omega S_0^I \sum_{m=1}^{\infty} m K_m^{\text{CoM}} \right]}. \]  

(39)

Next, for the sum rule of second order we have instead

\[ S_2 = S_2^I \sum_{m=0}^{\infty} K_m^{\text{CoM}} + \Omega^2 S_0^I \left[ K_1^{\text{CoM}} + K_2^{\text{CoM}} m^2 + \ldots \right] + 2\Omega S_1^I \left[ K_1^{\text{CoM}} + K_2^{\text{CoM}} m^2 + \ldots \right] \]  

(40)

\[ = S_2^I \sum_{m=0}^{\infty} K_m^{\text{CoM}} + S_1^I \sum_{m=1}^{\infty} m K_m^{\text{CoM}} + S_0^I \Omega^2 \sum_{m=1}^{\infty} m^2 K_m^{\text{CoM}}, \]

so that the intrinsic sum rule of second order can be obtained as

\[ S_2^I = \frac{1}{\sum_{m=0}^{\infty} K_m^{\text{CoM}} \left[ S_2 - S_1^I 2\Omega \sum_{m=1}^{\infty} m K_m^{\text{CoM}} - S_0^I \Omega^2 \sum_{m=1}^{\infty} m^2 K_m^{\text{CoM}} \right]}. \]  

(41)

Finally, for a generic sum rule of order \( n \) we have

\[ S_n = K_0^{\text{CoM}} S_n^I + \sum_{k=0}^{n} \binom{n}{k}(\Omega)^{n-k} S_k^I \sum_{m=1}^{\infty} K_m^{\text{CoM}} m^{-n-k} = K_0^{\text{CoM}} S_n^I + S_n^I \sum_{m=1}^{\infty} K_m^{\text{CoM}} + \sum_{k=0}^{n-1} \binom{n}{k}(\Omega)^{n-k} S_k^I \sum_{m=1}^{\infty} K_m^{\text{CoM}} m^{-n-k}, \]  

(42)

\[ = S_n^I \sum_{m=0}^{\infty} K_m^{\text{CoM}} + \sum_{k=0}^{n-1} \binom{n}{k}(\Omega)^{n-k} S_k^I \sum_{m=1}^{\infty} K_m^{\text{CoM}} m^{-n-k}, \]

and the intrinsic sum rule of order \( n \) can be found as

\[ S_n^I = \frac{1}{\sum_{m=0}^{\infty} K_m^{\text{CoM}} \left[ S_n - \sum_{k=0}^{n-1} \binom{n}{k}(\Omega)^{n-k} S_k^I \sum_{m=1}^{\infty} K_m^{\text{CoM}} m^{-n-k} \right]}. \]  

(43)

This is the second important recursive equation resulting from our formalism.

IV. ELECTRON SCATTERING PROCESS

We now direct our attention to an application of the newly derived formalism to a chosen physical scattering process that serves as an example. In the inclusive electron scattering off an \( A \)-body nucleus, one deals with two kind of electromagnetic response functions, namely the longitudinal and the transverse response function. Here we will consider the former, which involves the charge operator

\[ \hat{O} = \sum_{k=1}^{Z} e^{i\mathbf{q}\mathbf{r}_k}, \]  

(44)

where \( \mathbf{r}_k \) is the coordinate of each nucleon in the laboratory frame, \( \mathbf{q} \) is the momentum transfer from the electron to the nucleus and \( Z \) is the number of protons in the nu-
multipoles, respectively. The CoM wave function is formed with projection factors. The multipole expansions of the CoM and intrinsic coordinates in plane waves read [25]

\[ e^{i \mathbf{q} \mathbf{R}_{\text{CoM}}} = 4\pi \sum_{\mathbf{R}} i^{J} j(J, \mathbf{R}) Y_{JM}(\mathbf{R}) \mathbf{C}_{JM}(\mathbf{q}), \]

and

\[ \sum_{k=1}^{Z} e^{i \mathbf{q} \mathbf{r}_{k}} = 4\pi \sum_{\mathbf{R}} i^{J} \sum_{k=1}^{Z} j(J, \mathbf{R}) Y_{jm}(\mathbf{R}) Y_{jm}(\mathbf{q}), \]

where \( \mathbf{C}_{JM} \) and \( \mathbf{C}_{jm} \) are the CoM and intrinsic Coulomb multipole amplitudes, respectively. The CoM wave function is a harmonic oscillator state, written in general as

\[ \psi_{\text{CoM}}^{MN}(\mathbf{R}) = R_{N,r}(\mathbf{R}) Y_{LM}(\mathbf{R}), \]

with energy \( E = h\Omega(N + \frac{1}{2}) \) where \( N = 2N_{r} + J \) and \( J \leq N \). In the ground state, the oscillator wave function has the quantum numbers \( N_{r} = 0, J_{0} = 0, M_{0} = 0 \) so that the initial state will be

\[ \psi_{000}(\mathbf{R}) = \sqrt{\frac{2}{4\pi b_{\text{CoM}}^{3}}} \times e^{-\frac{\mathbf{r}^{2}}{2b_{\text{CoM}}^{2}}}, \]

where \( b_{\text{CoM}} = \sqrt{\frac{\hbar}{\Delta M N \Omega}} \) is the harmonic oscillator length.

Our formalism requires the knowledge of the CoM transition probabilities of Eq. (20) for the CoM Coulomb operator \( \mathbf{C}_{JM} \). Since it carries angular momentum \( J \) with projection \( M \) and the quantum numbers of the initial CoM state are all zero, obviously the final state quantum numbers and wave function will be [28]

\[ \psi_{NJM}(\mathbf{R}) = R_{N,r}(\mathbf{R}) Y_{JM}(\mathbf{R}), \]

where

\[ \begin{align*}
\psi_{NJM}(\mathbf{R}) &= \sqrt{\frac{2}{4\pi b_{\text{CoM}}^{3}}} \times e^{-\frac{\mathbf{r}^{2}}{2b_{\text{CoM}}^{2}}} Y_{JM}(\mathbf{R}), \\
&\times e^{-\frac{\mathbf{r}^{2}}{2b_{\text{CoM}}^{2}}} L_{N_{r}}^{2} \left( \frac{R_{\text{CoM}}}{b_{\text{CoM}}} \right)^{J} Y_{JM}(\mathbf{R}).
\end{align*} \]

Starting from Eq. (20) and using Eq. (46) and (47) for \( \mathbf{O}_{\text{CoM}} \) we obtain

\[ K_{N}^{\text{CoM}} = \sum_{JM} \left| \langle \psi_{NJM}^{\text{CoM}} | \mathbf{O}_{\text{CoM}} | \psi_{000}^{\text{CoM}} \rangle \right|^{2}, \]

where the sum over \( J' \) and \( M' \) is dropped due to selection rules. Using the Wigner-Eckart theorem [25], the matrix elements of \( \mathbf{C}_{JM} \) can be related to that with angular momentum projection \( M = 0 \), so that essentially one only needs \( \langle \psi_{NJM}^{\text{CoM}} | \mathbf{C}_{JM}^{\text{CoM}} | \psi_{000}^{\text{CoM}} \rangle \). The latter turns out to be expressed in terms of the Gamma’s and Kummer’s functions (\( M \)) as [29, 30]

\[ \langle \psi_{NJM}^{\text{CoM}} | \mathbf{C}_{JM}^{\text{CoM}} | \psi_{000}^{\text{CoM}} \rangle = \frac{i^{J} \times \sqrt{\sqrt{4\pi^{(2J+1)}}^{(2N_{r}+J+1/2)} \Gamma(N_{r}+1)} \left( \frac{b_{h\mathbf{O} = 20\text{ MeV}}}{} \right)^{J}}{2(2J+1)!} \times \sum_{m=0}^{N_{r}} (-1)^{m} \frac{1}{(N_{r}+m+1)!} P_{jm}(\Omega) \times M \left( J + \frac{3}{2} + m, J + \frac{3}{2} - \frac{b_{\text{CoM}}^{2}}{2} \right). \]

Details for the analytical derivation are found in Appendix A. Using Eq. (52) and Eq. (A12) one can write down the first CoM transition probabilities as

\[ K_{N}^{\text{CoM}} = \sum_{JM} \left| \langle \psi_{NJM}^{\text{CoM}} | \mathbf{O}_{\text{CoM}} | \psi_{000}^{\text{CoM}} \rangle \right|^{2}, \]

which we plot for the first few \( N \) in Fig. 1 for \( h\Omega = 20\text{ MeV} \). We have numerically verified that Eq. (21) holds true. These expressions of the CoM transition probabilities have already been used in Ref. [31] to analyze the CoM contamination of coupled-cluster theory calculations of the Coulomb sum rule.

V. THE PHOTOOBSORPTION PROCESS

We now turn our attention to another example, namely the photoabsorption process, i.e., the absorption of a real photon by a nucleus. In this case we have a relation between the energy transfer and the momentum transfer, namely \( \omega = |\mathbf{q}| \). In the low-energy regime the leading
response function is the so called unretarded dipole response function [19, 32, 33] and the $z$-component of the dipole operator can be written as

$$
\hat{D}_z = \sum_{i=1}^Z z_k, \quad (55)
$$

where $z_k$ is the $z$-component of the $k$-th particle coordinate in the laboratory frame. Clearly, in this case, if we use the relative coordinate $z_k = z_k - Z_{\text{CoM}}$, we are not in a situation in which the operator factorizes as in Eq. (8), but rather we have an operator that is the sum of the CoM and intrinsic part as

$$
\hat{O} = \hat{O}^I + \hat{O}^{\text{CoM}}. \quad (56)
$$

Hence, we cannot immediately apply our formula in Eqs. (27) and (43). It is therefore necessary to extend our formalism. For this purpose, we write

$$
\hat{O}^I + \hat{O}^{\text{CoM}} = \frac{d}{dx} \left( e^{\alpha \hat{O}^I} \hat{O}^{\text{CoM}} \right) \bigg|_{\alpha = 0} \quad (57)
$$

and reduce the problem to the ansatz of Eq. (8) $\hat{O} = \hat{O}^I \hat{O}^{\text{CoM}}$ with the operators $\hat{O}^I$ and $\hat{O}^{\text{CoM}}$ that depend on the parameter $\alpha$.

We will now focus on the dipole response function and consider the nuclear two-body problem ($A = 2$) to obtain a proof of principle of our formalism. In case of the deuteron, composed by a proton and a neutron, we only have one charged particle. Its $z$-component is denoted with $z_1$, so that the dipole operator of Eq. (55) becomes

$$
\hat{D}_z = z_1 = \frac{z}{2} + Z_{\text{CoM}}. \quad (58)
$$

We define

$$
\hat{O}^I \equiv e^{\alpha \hat{D}_z}, \quad \hat{O}^{\text{CoM}} \equiv e^{\alpha Z_{\text{CoM}}}, \quad (59)
$$

so that these operators become

$$
\hat{O}^I \approx 1 + \alpha \frac{z}{2} = 1 + \alpha z' = 1 + \alpha \hat{O}^I, \quad (60)
$$

$$
\hat{O}^{\text{CoM}} \approx 1 + \alpha Z_{\text{CoM}} = 1 + \alpha \hat{O}^{\text{CoM}}
$$

for small $\alpha$, where the relative coordinate in the two-body intrinsic frame is $z' = \frac{z_1 - z_2}{2}$ and $Z_{\text{CoM}} = \frac{z_1 + z_2}{2}$. In this way, we obtain that

$$
\hat{O} = \hat{O}^I \hat{O}^{\text{CoM}} = \left( 1 + \alpha \frac{z_1 - z_2}{2} \right) \left( 1 + \alpha \frac{z_1 + z_2}{2} \right) \quad (61)
$$

$$
\hat{O} = \hat{O}^I \hat{O}^{\text{CoM}} = \frac{1}{2} \left( z_1 + \frac{\alpha}{2} \frac{z_1 - z_2}{2} \right) \left( z_2 + \frac{\alpha}{2} \frac{z_1 + z_2}{2} \right).
$$

Considering the operators $\hat{O}^I$ in the intrinsic frame and $\hat{O}$ in the laboratory frame, we define the respective sum rules of order $n$ as $S^I_n$ and $S_n$. From Eq. (43), we obtain that the relations between the sum rule of the first three orders ($n = 0, 1, 2$) are

$$
\tilde{S}^I_0 = \frac{\tilde{S}_0}{\sum_{N=0}^\infty K_N^{\text{CoM}}}, \quad (62)
$$

$$
\tilde{S}^I_1 = \tilde{S}_1 - \Omega \tilde{S}^I_0 \sum_{N=0}^\infty K_N^{\text{CoM}}, \quad (63)
$$

$$
\tilde{S}^I_2 = \tilde{S}_2 - 2\Omega \tilde{S}_1 \sum_{N=0}^\infty N K_N^{\text{CoM}} - \Omega^2 \tilde{S}^I_0 \sum_{N=0}^\infty N^2 K_N^{\text{CoM}}.
$$

We now calculate the CoM transition probabilities $K_N^{\text{CoM}}$. Details are worked out in Appendix B, leading to

$$
K_0^{\text{CoM}} = |\langle \tilde{\psi}_{000} | \tilde{O}^{\text{CoM}} | \tilde{\psi}_{000} \rangle|^2 = 1, \quad (64)
$$

$$
K_1^{\text{CoM}} = |\langle \tilde{\psi}_{010} | \tilde{O}^{\text{CoM}} | \tilde{\psi}_{000} \rangle|^2 = \frac{\alpha b_{\text{CoM}}^2}{2}, \quad (65)
$$

$$
K_2^{\text{CoM}} = 0, \quad \text{for} \quad N \geq 2,
$$

where here again $b_{\text{CoM}}$ is the CoM harmonic oscillator length (this time with mass equal to $2m_N$). We observe then that

$$
\sum_{N=0}^\infty K_N^{\text{CoM}} = 1 + \frac{\alpha^2 b_{\text{CoM}}^2}{2}. \quad (66)
$$

With the help of Eq. (64), the relation between the sum rules of order $n = 0$ becomes

$$
\tilde{S}_0 = \frac{1}{1 + \frac{\alpha^2 b_{\text{CoM}}^2}{2}} \left[ \tilde{S}_1 - \Omega \tilde{S}_0 \frac{\alpha^2 b_{\text{CoM}}^2}{2} \right], \quad (67)
$$

and

$$
\tilde{S}_2 = \frac{1}{1 + \frac{\alpha^2 b_{\text{CoM}}^2}{2}} \left[ \tilde{S}_2 - 2\Omega \tilde{S}_1 \frac{\alpha^2 b_{\text{CoM}}^2}{2} - \Omega^2 \tilde{S}_0 \frac{\alpha^2 b_{\text{CoM}}^2}{2} \right]. \quad (68)
$$

The intrinsic operator $\hat{O}^I$ is simply related to the standard (translational invariant) unretarded dipole operator $\hat{O}^I = z'$, see (60). Denoting with $S^I_n$ the corresponding sum rules of order $n$, it is not difficult to establish the following relations

$$
\tilde{S}^I_0 = 1 + \alpha^2 S^I_0 \quad \text{for} \quad n = 0
$$

$$
\tilde{S}^I_n = \alpha^2 S^I_n \quad \text{for higher} \quad n. \quad (69)
$$

These are the other two equations we want to verify.
A. Numerical implementation

At this point we can verify our formalism with a numerical implementation by checking Eqs. (65) and (68), where for the l.h.s. of the latter we will exploit (66) and (67). To this purpose we use a modern nucleon-nucleon interaction stemming from chiral effective field theory at next-to-next-to-next-to-leading order \[34\], called N^3LO-EM, and solve the two-body problem using a harmonic oscillator basis. We use either the intrinsic frame, where the task reduces to the solution of a one-body problem in the relative coordinate, or in the laboratory frame where we have a two-body problem in the two single-particle coordinates.

Before dealing with our new formalism, we first check our numerical implementation, computing the deuteron ground-state energy \(\varepsilon_0\). In Fig. 2, we show the energy calculated in the intrinsic frame and laboratory frame for \(N_{\text{max}}\) up to 40 and different \(\hbar \Omega\). We get a perfect match between both calculations for every model space. As expected we see that, as \(N_{\text{max}}\) grows, the energies approach the converged values from above due to the variational principle. At \(N_{\text{max}} = 40\) for \(\hbar \Omega = 16\) MeV we obtain \(\varepsilon_0 = -2.2236\) MeV, which is rather close to the experimental value \(\varepsilon_{0}^{\exp} = -2.224573(2)\) MeV \[35\]. However, the goal of this paper is not necessarily to compare with experiment, but rather to compare calculations in the intrinsic \[36\] and laboratory frames \[37\].

Next we implement the dipole operators \[37\] so we are ready to numerically verify our formalism. In Fig. 3, we plot the l.h.s. of Eq. (65), calculated numerically, against the expected analytical behavior. For every \(\alpha\) we obtain agreement within \(10^{-3} - 10^{-4}\). To get an ever better agreement one needs to increase the model space size \(N_{\text{max}}\) so that the sum rules are fully converged. However, in the laboratory frame the size of the Hamiltonian matrix is very large (few GB for \(N_{\text{max}} = 40\) compared to few MB in the intrinsic frame for \(N_{\text{max}} = 300\)), hence we stop at \(N_{\text{max}} = 40\) since the test is sufficient to prove that Eq. (65) is numerically correct.

Next, for the sum rules of order \(n = 0, 1, 2\), we want to verify Eq. (68). To this purpose, we divide the l.h.s. by the r.h.s. of this equation and plot the ratio \(f = \frac{\text{l.h.s.}}{\text{r.h.s.}}\) as a function of \(N_{\text{max}}\) in Fig. 4. We clearly see that the ratio converges to 1 when the model space gets large enough, proving that Eq. (66) and (67) are numerically verified. This constitutes a proof of principle that the relations we derived are correct. Therefore they can be used for other operators than the dipole in order to extract intrinsic properties from laboratory frame calculations.

VI. CONCLUSIONS

In this paper we derive a new formalism to extract intrinsic response functions and sum rules from calculations performed in a general frame. The derivation is based on the use of a harmonic oscillator to confine the
The spherical Bessel function can be written in terms of the Bessel function.

The angular part of the integral is exactly the orthogonality relation of spherical harmonics, thus equal to 1. The energy excitation regime of about 20 MeV, which is the range of the giant dipole resonance.

Finally, we would like to point out that this formalism may be of great benefit for calculations of electroweak properties for nuclei beyond $A = 2$, in particular in the $s$- and $p$-shell nuclei, which owing to their light mass, are mostly affected by the center of mass effects. Applications to other nuclei will be explored in the future.

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Appendix A: CoM transition matrix elements for the Coulomb operator

Below we show the derivation of the CoM transition matrix element in case of the Coulomb operator, see Eq. (46) and (47). Using the same initial and final wave functions of Eqs. (50) and (51) one can analytically calculate the CoM matrix element as [30]

\[\begin{align*}
\langle \Psi_{NJM}^{\text{CoM}}|\hat{C}_{JM}\Psi_{000}^{\text{CoM}} \rangle &= \iiint dR_{\text{CoM}} \sin \theta d\theta d\varphi R_{\text{CoM}}^2 \sqrt{\frac{2N_r!}{b_{\text{CoM}}^3}} \left(\frac{R_{\text{CoM}}}{b_{\text{CoM}}}\right)^J e^{\frac{R_{\text{CoM}}^2}{2b_{\text{CoM}}^2}} \\
&\times L_{N_J}^{J+\frac{1}{2}} \left(\frac{R_{\text{CoM}}^2}{b_{\text{CoM}}^2}\right) Y_{J_M}^* (\hat{R}_{\text{CoM}}) 4\pi i^J \frac{j_j(qR_{\text{CoM}})}{\Gamma(N_r + J + 3/2)} Y_{J_M} (\hat{R}_{\text{CoM}}) \sqrt{\frac{2}{4\pi b_{\text{CoM}}^3 \Gamma(3/2)}} e^{\frac{q^2 b_{\text{CoM}}^2}{2}} \\
&\times \int dR_{\text{CoM}} R_{\text{CoM}}^2 \left(\frac{R_{\text{CoM}}}{b_{\text{CoM}}}\right)^J e^{- \frac{R_{\text{CoM}}^2}{b_{\text{CoM}}^2}} L_{N_J}^{J+\frac{1}{2}} \left(\frac{R_{\text{CoM}}^2}{b_{\text{CoM}}^2}\right) j_j(qR_{\text{CoM}}) \ .
\end{align*}\]

The angular part of the integral is exactly the orthogonality relation of spherical harmonics, thus equal to 1. The spherical Bessel function can be written in terms of the Bessel function [38]

\[j_j(qR_{\text{CoM}}) = \sqrt{\frac{\pi}{2q}} R_{\text{CoM}}^{\frac{J+1}{2}} j_{J+\frac{1}{2}}(qR_{\text{CoM}}) .\]

The Laguerre polynomials are finite degree polynomials expressed by [38]

\[L_N^\alpha(x) = \sum_{m=0}^{N} (-)^m \binom{N_r + \alpha}{N - m} \frac{1}{m!} x^m ,\]

so that

\[L_{N_J}^{J+\frac{1}{2}} \left(\frac{R_{\text{CoM}}^2}{b_{\text{CoM}}^2}\right) = \sum_{m=0}^{N_r} (-)^m \binom{N_r + J + \frac{1}{2}}{N_r - m} \frac{1}{m!} \left(\frac{R_{\text{CoM}}^2}{b_{\text{CoM}}^2}\right)^m .\]
Substituting the latter into our expression for the matrix element we obtain

\begin{align}
\langle \Psi_{NJM}^{\text{CoM}} | C_{JM}^{\text{CoM}} | \Psi_{000}^{\text{CoM}} \rangle & = \frac{4}{b_{\text{CoM}}^4} \sqrt{\frac{\pi N_r!}{\Gamma(N_r + J + 3/2) \Gamma(3/2)}} i^{J} Y_{JM}^{*}(\mathbf{q}) \int dR_{\text{CoM}} R_{\text{CoM}}^{2} \left( \frac{R_{\text{CoM}}}{b_{\text{CoM}}} \right)^{J} e^{-\frac{b_{\text{CoM}}^{2}}{4}} \\
& \times \left[ \sum_{m=0}^{N_r} (-1)^{m} \frac{(N_r + J + \frac{1}{2})}{N_r - m} \frac{1}{m!} \left( \frac{R_{\text{CoM}}^{2}}{b_{\text{CoM}}^{2}} \right)^{m} \right] \left[ \sqrt{\frac{\pi}{2q}} R_{\text{CoM}}^{1/2} J_{J+M}^{1/2} \left( q R_{\text{CoM}} \right) \right] \\
& = \frac{4}{b_{\text{CoM}}^4} \sqrt{\frac{\pi N_r!}{\Gamma(N_r + J + 3/2) \Gamma(3/2)}} i^{J} Y_{JM}^{*}(\mathbf{q}) \sum_{m=0}^{N_r} (-1)^{m} \frac{(N_r + J + \frac{1}{2})}{N_r - m} \frac{1}{m!} b_{\text{CoM}}^{-2m-J} \sqrt{\frac{\pi}{2q}} \\
& \times \int dR_{\text{CoM}} R_{\text{CoM}}^{2} R_{\text{CoM}}^{J+2m} e^{-\frac{b_{\text{CoM}}^{2}}{4}} J_{J+\frac{1}{2}}(q R_{\text{CoM}}) .
\end{align}

To calculate the integral

\begin{equation}
\int dR_{\text{CoM}} R_{\text{CoM}}^{J+2m} e^{-\frac{b_{\text{CoM}}^{2}}{4}} J_{J+\frac{1}{2}}(q R_{\text{CoM}})
\end{equation}

we can use equation (11.428) in Ref. [38]

\begin{equation}
\int_{0}^{\infty} x^{\mu-1} e^{-ax^2} J_{\nu}(cx) dx = \frac{\Gamma\left(\frac{\nu}{2} + \frac{\mu}{2}\right)}{2a^{\mu}\Gamma(\nu + 1)} M \left( \frac{1}{2} \nu + \frac{1}{2} \mu + 1, -\frac{c^2}{4a^2} \right).
\end{equation}

The Kummer’s function $M$ is

\begin{equation}
M(a, b, x) = 1 + \frac{ax}{b} + \frac{a(a+1)x^2}{b(b+1)2!} + \frac{a(a+1)(a+2)x^3}{(b)(b+1)(b+2)3!} + \ldots + \frac{(a)_{n}x^n}{(b)_{n}n!} + \ldots,
\end{equation}

where $(a)_{n} = a(a+1)(a+2)\ldots(a+n-1)$ and similarly $(b)_{n}$. We define

\begin{equation}
\mu \equiv J + \frac{5}{2} + 2m, \quad a \equiv \frac{1}{b}, \quad \nu \equiv J + \frac{1}{2}, \quad c \equiv q, \quad x \equiv R_{\text{CoM}},
\end{equation}

and we can write the result of Eq. (A6) as

\begin{equation}
\int dR_{\text{CoM}} R_{\text{CoM}}^{J+\frac{1}{2}+2m} e^{-\frac{b_{\text{CoM}}^{2}}{4}} J_{J+\frac{1}{2}}(q R_{\text{CoM}}) = \frac{\Gamma(J + \frac{3}{2} + m)(\frac{1}{2}q b_{\text{CoM}})^{J+\frac{1}{2}}}{2 b_{\text{CoM}}^{J+\frac{1}{2}+2m} \Gamma(J + \frac{3}{2})} \times M \left( J + \frac{3}{2} + m, J + \frac{3}{2}, -\frac{b_{\text{CoM}}^{2}q^{2}}{4} \right).
\end{equation}

Finally, we collect all the terms and rewrite Eq. (A5) obtaining the following expression

\begin{align}
\langle \Psi_{NJM}^{\text{CoM}} | C_{JM}^{\text{CoM}} | \Psi_{000}^{\text{CoM}} \rangle & = \frac{4}{b_{\text{CoM}}^4} \sqrt{\frac{\pi N_r!}{\Gamma(N_r + J + 3/2) \Gamma(3/2)}} i^{J} Y_{JM}^{*}(\mathbf{q}) \sum_{m=0}^{N_r} (-1)^{m} \frac{(N_r + J + \frac{1}{2})}{N_r - m} \frac{1}{m!} b_{\text{CoM}}^{-2m-J} \\
& \times \sqrt{\frac{\pi}{2q}} \frac{\Gamma(J + \frac{3}{2} + m)(\frac{1}{2}q b_{\text{CoM}})^{J+\frac{1}{2}}}{2 b_{\text{CoM}}^{J+\frac{1}{2}+2m} \Gamma(J + \frac{3}{2})} M \left( J + \frac{3}{2} + m, J + \frac{3}{2}, -\frac{b_{\text{CoM}}^{2}q^{2}}{4} \right).
\end{align}

Thus, the CoM matrix element of the Coulomb multipole becomes

\begin{align}
\langle \Psi_{NJM}^{\text{CoM}} | C_{JM}^{\text{CoM}} | \Psi_{000}^{\text{CoM}} \rangle & = i^{J} \sqrt{\frac{\pi}{\Gamma(N_r + J + 3/2) \Gamma(3/2)}} \frac{1}{2} q b_{\text{CoM}}^{J} \left( Y_{ JM}^{*}(\mathbf{q}) \right) \\
& \times \sum_{m=0}^{N_r} (-1)^{m} \frac{(N_r + J + \frac{1}{2})}{N_r - m} \frac{1}{m!} \frac{\Gamma(J + \frac{3}{2} + m)}{\Gamma(J + \frac{3}{2})} M \left( J + \frac{3}{2} + m, J + \frac{3}{2}, -\frac{b_{\text{CoM}}^{2}q^{2}}{4} \right).
\end{align}

We are free to choose the coordinate system parallel to the scattering direction $\mathbf{q}$, therefore the arguments of the spherical harmonic will be $\theta = \varphi = 0$. Knowing that

\begin{equation}
Y_{JM}^{*}(0,0) = \sqrt{\frac{2J + 1}{4\pi}} \delta_{M0},
\end{equation}
we can proceed only with $M = 0$, obtaining

$$
\langle \Psi_{N,0}^{\text{CoM}} | C_{J0}^{\text{CoM}} | \Psi_{000}^{\text{CoM}} \rangle = i^J \sqrt{\frac{N_r!}{\Gamma(N_r + J + 3/2) \Gamma(3/2)}} \left( \frac{1}{2} \delta_{\text{CoM}} \right)^J \sqrt{\frac{\pi(2J + 1)}{4}}
\times \sum_{m=0}^N (-1)^m \frac{(N_r + J + \frac{1}{2})}{N_r - m} \frac{\Gamma(J + \frac{3}{2} + m)}{\Gamma(J + \frac{3}{2}) m!} M \left( J + \frac{3}{2} + m, J + \frac{3}{2} - \frac{b_{\text{CoM}}^2 q^2}{4} \right).
$$

(A12)

Note that the phase $i^J$ is not important since we are looking at the squared modulus. Finally, using the properties of the gamma function we obtain

$$
\langle \Psi_{N,0}^{\text{CoM}} | C_{J0}^{\text{CoM}} | \Psi_{000}^{\text{CoM}} \rangle = i^J \sqrt{2J + 1} \frac{\Gamma(N_r + J + 3/2) \Gamma(N_r + 1)}{2 \Gamma^2(J + 3/2)} \left( \frac{b_{\text{CoM}} q^2}{2} \right)^J
\times \sum_{m=0}^N (-1)^m \frac{1}{(N_r - m + 1) \Gamma(m + 1)} M \left( J + \frac{3}{2} + m, J + \frac{3}{2} - \frac{b_{\text{CoM}}^2 q^2}{4} \right).
$$

(A13)

**Appendix B: CoM transition matrix elements for the dipole operator**

Below we show the derivation of the CoM transition matrix element in case of the $\alpha$-dependent operator of Eq. (60)

$$
K_N^{\text{CoM}} = \sum_{J_M} \left| \langle \Psi_{N,M}^{\text{CoM}} | \hat{O}^{\text{CoM}} | \Psi_{000}^{\text{CoM}} \rangle \right|^2,
$$

(B1)

with

$$
\hat{O}^{\text{CoM}} = 1 + \alpha \sqrt{\frac{4\pi}{3}} R_{\text{CoM}} Y_{10}(\hat{R}_{\text{CoM}}).
$$

(B2)

The CoM matrix element becomes

$$
\langle \Psi_{N,M}^{\text{CoM}} | \hat{O}^{\text{CoM}} | \Psi_{000}^{\text{CoM}} \rangle = \int_0^\infty dR_{\text{CoM}} R_{\text{CoM}}^3 \int d\hat{R}_{\text{CoM}} \left[ \frac{2N_r!}{b_{\text{CoM}}^3 \Gamma(N_r + J + 3/2)} \frac{(R_{\text{CoM}}^{\text{CoM}})^J e^{-\frac{\pi^2}{2 b_{\text{CoM}}^2} L_{J \frac{3}{2}}}}{\Gamma(J + \frac{3}{2})} \right]
\times Y_{J_M}^{*}(\hat{R}_{\text{CoM}}) \left[ 1 + \alpha \sqrt{\frac{4\pi}{3}} R_{\text{CoM}} Y_{10}(\hat{R}_{\text{CoM}}) \right] \frac{2}{b_{\text{CoM}}^3 \Gamma(3/2)} e^{-\frac{\pi^2}{2 b_{\text{CoM}}^2} L_{J \frac{3}{2}}}
\times \left( \delta_{J0} \delta_{M0} + \frac{\alpha}{\sqrt{3}} R_{\text{CoM}} \delta_{J1} \delta_{M0} \right)
= \frac{4N_r!}{b_{\text{CoM}}^3 \Gamma(3/2) \Gamma(N_r + J + 3/2)} \sum_{m=0}^N (-1)^m \frac{(N_r + J + \frac{3}{2})}{m!} \frac{1}{b_{\text{CoM}}^2}
\times \left( \delta_{J0} \delta_{M0} + \frac{\alpha}{\sqrt{3}} R_{\text{CoM}} \delta_{J1} \delta_{M0} \right)
\times \int_0^\infty dR_{\text{CoM}} R_{\text{CoM}}^{2m+J+2} e^{-\frac{\pi^2}{2 b_{\text{CoM}}^2} L_{J \frac{3}{2}}}
\times \frac{\Gamma(N_r + J + 1)}{\Gamma(3/2) \Gamma(N_r + J + 3/2)} \sum_{m=0}^N (-1)^m \frac{(N_r + J + \frac{3}{2})}{m!} \frac{1}{b_{\text{CoM}}^2}
\times \left( \Gamma\left( \frac{2m + J + 3}{2} \right) \delta_{J0} \delta_{M0} + \frac{\alpha b_{\text{CoM}}}{\sqrt{3}} \Gamma\left( \frac{2m + J + 4}{2} \right) \delta_{J1} \delta_{M0} \right).
$$

(B3)
From the previous result we see that only the matrix elements with \( M = 0 \) and \( J = 0, 1 \) are different from zero. They can finally be written as

\[
\langle \Psi_{N00}^{\text{CoM}} | \hat{O} | \Psi_{000}^{\text{CoM}} \rangle = \sqrt{\frac{2\Gamma(N_r + 1)\Gamma(N_r + 3/2)}{\sqrt{\pi}}} \sum_{m=0}^{N_r} (-1)^m \frac{1}{\Gamma(N_r - m + 1)\Gamma(m + 1)},
\]

(B4)

\[
\langle \Psi_{N10}^{\text{CoM}} | \hat{O} | \Psi_{000}^{\text{CoM}} \rangle = \alpha b_{\text{CoM}} \sqrt{\frac{2\Gamma(N_r + 1)\Gamma(N_r + 5/2)}{3\sqrt{\pi}}} \sum_{m=0}^{N_r} (-1)^m \frac{1}{\Gamma(N_r - m + 1)\Gamma(m + 1)}.
\]

(B5)

Now we want to evaluate the sum that occurs in the previous equations. To do this we consider the binomial coefficients \((x + y)^n = \sum_{k=0}^{n} \binom{n}{k} x^{n-k} y^k\) with \( x = 1 \) and \( y = -1 \), which give (for \( n \geq 1 \))

\[
0 = \sum_{k=0}^{n} (-1)^k \binom{n}{k} = n! \sum_{k=0}^{n} (-1)^k \frac{1}{(n-k)!} \Rightarrow \sum_{k=0}^{n} (-1)^k \frac{1}{(n-k)!} k! = 0.
\]

(B7)

We finally obtain the following results for the transition probabilities

\[
K_0^{\text{CoM}} = |\langle \Psi_{000}^{\text{CoM}} | \hat{O} | \Psi_{000}^{\text{CoM}} \rangle|^2 = 1,
\]

(B8)

\[
K_1^{\text{CoM}} = |\langle \Psi_{010}^{\text{CoM}} | \hat{O} | \Psi_{000}^{\text{CoM}} \rangle|^2 = \frac{\alpha^2 b_{\text{CoM}}^2}{2},
\]

(B9)

\[
K_N^{\text{CoM}} = 0, \quad N \geq 2.
\]

(B10)

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