Study of Nuclear Clustering from an *Ab Initio* Perspective

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We put forward a new *ab initio* approach that seamlessly bridges the structure, clustering, and reactions aspects of the nuclear quantum many-body problem. The configuration interaction technique combined with the resonating group method based on a harmonic oscillator basis allows us to treat the reaction and multiclustering dynamics in a translationally invariant way and preserve the Pauli principle. Our presentation includes studies of ^{8,10}Be and an exploration of 3α clustering in ^{12}C.

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The unified description of many-body nuclear structure and reactions from fundamental, *ab initio*, principles is a central issue in modern nuclear physics, astrophysics, and mesoscopic quantum physics, in general. Challenging questions about the role of intrinsic degrees of freedom in nuclear reactions [1,2], the emergence of rotational behavior in the continuum [3,4], the interplay between structure, reactions, and the single-particle and collective motion in nuclear states [5,6], near-threshold clustering effects [7–10], large-amplitude collective motion and shape coexistence [11], and the phenomenon of superradiance, where structural clustering is enhanced or reduced due to reaction dynamics [12], still remain.

The recent decades have seen outstanding progress in methods related to both nuclear structure [13–17] and nuclear reactions [18–23]; however, a unified treatment of the two remains challenging. For two-body processes, there is a wealth of strategies that solve the structure-reaction problems: matching solutions [21,24], the R-matrix method [25], Hilbert space projection techniques such as the shell model embedded in the continuum (SMEC) [26] or the continuum shell model (CSM) [19], the Berggren complex-plane formulation [27], Lüscher's finite-volume method [20,28], or the HORSE (J-matrix) formalism [29,30]. However, the coupling between intrinsic structure and the continuum of reaction states remains a particularly difficult question when it comes to multiple final-state fragments, decay fragments with complex internal structures [2], long-range interactions [31], competing direct and sequential decay modes [32,33], or many open channels that are equally significant and provide a structural feedback from the continuum [12]. These problems are not unique to nuclear physics, as they are encountered in many branches of physics related to open mesoscopic quantum systems: quantum information [34], electronic transport [35], quantum optics [36], biological light-harvesting complexes [37], and plasmonic antenna arrays [38], to name a few.

In this work, we put forward a novel strategy that bridges the *ab initio* configuration interaction structure calculations with reactions through a resonating group method (RGM) [39]. The RGM provides a general formal strategy for coupling asymptotic reaction states and cluster degrees of freedom with the intrinsic structure needed to apply methods such as R matrix, CSM, or SMEC [19,22,40,41]. In order to overcome the previously mentioned impediments and limitations, we propose to build RGM multicluster channels using a harmonic oscillator (HO) basis expansion of the relative motion between fragments. These intrinsic channel states coupled with asymptotic solutions provide the needed structure-reaction interface.

We operate here with the multinucleon shell-model-type wave functions Ψ, which are linear combinations of Slater determinants of the single-particle HO states. We use the formalism of second quantization, which preserves the antisymmetry and allows us to view the many-body state as a many-body creation operator that creates this state from the vacuum; constructions of the type $|\Psi(1)\Psi(2)\rangle \equiv \hat{\Psi}^\dagger(2)\hat{\Psi}^\dagger(1)|0\rangle$ are automatically antisymmetrized [42].

The HO basis adopted for this work allows for a formal separation of the center-of-mass (c.m.) degrees of freedom, leading to a translationally invariant approach. In both traditional shell model and no-core shell model (NCSM) approaches, where basis states are restricted by the maximum number of oscillator excitation quanta $N_{\max}$, the HO Hamiltonian for the c.m. can be used to factorize the c.m. degree of freedom in the many-body wave function [43], leading to physical states of interest being in the form

$$\Psi = \phi_{000}(\mathbf{R})\Psi'. \tag{1}$$

Here $\phi_{n\ell m}(\mathbf{R})$ denotes the HO wave function with n nodes, angular momentum ℓ, and magnetic projection m, while Ψ' is a translationally invariant function of relative coordinates only. For example, the $N_{\max} = 0$ structure of an α particle amounts to representing the wave function with a single Slater determinant containing two protons and two neutrons in the lowest $0s$ HO shell, sometimes called an s^4 structure. We denote this by $\alpha[0]$, where the $N_{\max}$ value appears in square brackets; we use this notation for the

remainder of the text. The c.m. motion of this $\alpha[0]$ structure is described by the lowest oscillator state $\phi_{000}(\mathbf{R})$. Given the compact nature of the α particle, the translationally invariant part of the simple $\alpha[0]$ wave function represents over 90% of the physical α, assuming a proper selection of the HO frequency around $\hbar\Omega \approx 25$–27 MeV. The $\alpha[0]$ approximation is commonly used in α clustering studies [42,44–46], as it allows for an algebraic treatment that utilizes the SU(3) symmetry of the isotropic HO.

In order to construct reaction channels in which clusters are moving relative to each other and the overall translational invariance is respected, we build "boosted" states

$$\Psi_{n\ell m} = \phi_{n\ell m}(\mathbf{R})\Psi', \tag{2}$$

where the c.m. can be in any desired oscillator state, while the intrinsic part Ψ' remains unchanged. We do this numerically without any approximations or truncations using the c.m. creation and annihilation operators, $\mathcal{B}^\dagger$ and $\mathcal{B}$ correspondingly. These vector operators are parts of the usual isoscalar dipole operator. Starting from $\Psi \equiv \Psi_{000}$ in Eq. (1), the number of nodes n can be increased with a scalar product $\mathcal{B}^\dagger \cdot \mathcal{B}^\dagger$, namely, $|\Psi_{n+1\ell m}\rangle \propto (\mathcal{B}^\dagger \cdot \mathcal{B}^\dagger)|\Psi_{n\ell m}\rangle$, while the c.m. angular momentum vector ℓ is proportional to a vector product $\mathcal{B}^\dagger \times \mathcal{B}$; and in practice a series of aligned $\ell = m$ states is obtained using the raising component $\mathcal{B}^\dagger_{m=+1}$. The total number of oscillator excitation quanta in (2) is shared between the c.m. and intrinsic degrees of freedom $N = N_{\text{c.m.}} + N'$, where $N_{\text{c.m.}} = 2n + \ell$; see also Ref. [47]. Many previous works [42,45,48,49] employed the $\alpha[0]$ approximation for the α particle, in which case the boosted states in Eq. (2) can be expressed analytically in the SU(3) HO basis.

Consider a reaction process $A_1 + A_2 = A$, where A_1 and A_2 are two fragments forming the parent system A. We construct, and correspondingly define, each reaction channel basis state $|\Phi_{n\ell J}\rangle$ as a linear combination of boosted, fully antisymmetrized states $|\Psi_{n_1\ell_1 m_1}(1)\Psi_{n_2\ell_2 m_2}(2)\rangle$ coupling their c.m. motions so that the two clusters A_1 and A_2 are in a relative HO state $\phi_{n\ell m}(\boldsymbol{\rho})$, where $\boldsymbol{\rho} = \mathbf{R}_1 - \mathbf{R}_2$, and the overall c.m. variable of the state is in the $N_{\text{c.m.}} = 0$ HO state that coincides with the c.m. state of the parent A. This coupling can be done using oscillator (Talmi-Moshinsky) brackets. The orbital angular momenta of c.m. motion are coupled as $\ell_1 + \ell_2 = \ell$, the total nuclear spins of each fragment $A_{1,2}$ are coupled as $\boldsymbol{J}_1 + \boldsymbol{J}_2 = \boldsymbol{S}$, and finally the combined intrinsic nuclear spin S and the angular momentum of relative motion ℓ give the total angular momentum of the channel $\ell + \boldsymbol{S} = \boldsymbol{J}$. We can write the basis channel state in abbreviated form as

$$|\Phi_{n\ell J}\rangle = |\{\phi_{000}(\mathbf{R})\phi_{n\ell m}(\boldsymbol{\rho})\{\Psi'(1)\Psi'(2)\}_S\}_J\rangle, \tag{3}$$

and the commutation rules of second quantization used in the construction process ensure full antisymmetrization.

TABLE I. Absolute values of spectroscopic amplitudes and channel norms for various types of parent states and basis channels. All channels here have $\ell = 0$, and the number of quanta in relative motion of the two fragments is denoted by $N_c = 2n + \ell$. For each nucleus, square brackets indicate the structure used for the corresponding fragment which could include spectroscopic notation, a pair of SU(3) quantum numbers, or $N_{\max}$ as a single integer.

Parent	Channel	N_c	$\lvert\langle\Psi\lvert\Phi_{n\ell J}\rangle\rvert$	$\langle\Phi_{n\ell J}\lvert\Phi_{n\ell J}\rangle$
^{16}O[0]	^{12}C[(0, 4)] + α[0]	4	$\sqrt{8/27}$	8/27
^{16}O[0]	^{12}C[$p^8_{3/2}$] + α[0]	4	0.135	0.018
^{16}O[0]	^{12}C[$p^8_{3/2}$] + α[4]	4	0.130	0.017
^{8}Be[(4, 0)]	α[0] + α[0]	4	$\sqrt{3/2}$	3/2
^{8}Be[0]	α[0] + α[0]	4	1.160	3/2
^{8}Be[4]	α[0] + α[0]	4	0.984	3/2
^{8}Be[4]	α[0] + α[0]	6	0.644	15/8
^{8}Be[4]	α[2] + α[2]	4	0.981	1.492
^{12}C[$p^8_{3/2}$]	α[0] + α[0] + α[0]	8	1/4	81/80
^{16}O[0]	$(\alpha[0])^4$	12	$\sqrt{3/10}$	3/10

The wave functions $|\Phi_{n\ell J}\rangle$ provide a convenient basis set for expanding the true cluster relative motion in terms of harmonic oscillator functions $\phi_{n\ell m}(\boldsymbol{\rho})$. The overlaps $\langle\Psi|\Phi_{n\ell J}\rangle$ are translationally invariant by construction, and their total norm $\text{SF} = \sum_n |\langle\Psi|\Phi_{n\ell J}\rangle|^2$, known as the traditional spectroscopic factor, provides the simplest spectroscopic clustering characteristic of states (1) of parent A, clustering into $A_1 + A_2$ fragments.

In Table I, we show select examples of spectroscopic overlaps for various systems and channels. The algebraic SU(3) examples and closed-shell limits confirm known analytic results [44,50,51]. The basis channels $\Phi_{n\ell J}$ are not normalized (see last column of Table I) nor generally orthogonal, which makes it hard to associate amplitudes in Table I and the corresponding traditional spectroscopic factors with observables. Thus, the renormalized spectroscopic factors [52] obtained as a result of the orthonormalization of the basis channels are commonly discussed [6,42].

There is no substantial change in our approach for channels with more than two fragments in the final state; Eq. (3) can be generalized using the same boosting procedure where c.m. motion is controlled via Jacobi coordinates or by using a generalization of the oscillator brackets obtained numerically using diagonalization, similar to the method in Ref. [53]. Multi-α channel examples are included in Table I.

Next we consider a full dynamical problem within the RGM framework. Here, the actual channel wave function for a given set of asymptotic quantum numbers (which in the following we abbreviate with a single label ℓ) is given as an expansion of basis channel states (3), enumerated with n:

$$\mathcal{F}_\ell(\rho) = \sum_n \chi_n \Phi_{n\ell}. \quad (4)$$

The form of this expansion is determined variationally using the generalized eigenvalue problem

$$\sum_n \mathcal{H}^{(\ell)}_{nn'} \chi_{n'} = E \sum_n \mathcal{N}^{(\ell)}_{nn'} \chi_{n'}, \quad (5)$$

where

$$\mathcal{H}^{(\ell)}_{nn'} = \langle \Phi_{n\ell} | H | \Phi_{n'\ell} \rangle \quad \text{and} \quad \mathcal{N}^{(\ell)}_{nn'} = \langle \Phi_{n\ell} | \Phi_{n'\ell} \rangle. \quad (6)$$

The channel normalization requires $\sum_n \mathcal{N}^{(\ell)}_{nn'} \chi^*_n \chi_{n'} = 1$. Now, the Hamiltonian is used to establish the reaction channels dynamically. For two-body reactions, the procedure amounts to an expansion of the relative motion in a HO basis, where the expansion index n is the number of nodes in the relative motion. For large n, which are associated with large relative separation of the two fragments, the basis channels $\Phi_{n\ell}$ become orthogonal and the matrix elements of the relative motion Hamiltonian are given by Coulomb and kinetic energy matrix elements that are known analytically.

In general, these intermediate-range RGM solutions should be properly matched or combined in the Hilbert space with the asymptotic ones through other techniques such as R matrix or CSM. For long-lived resonances, the continuum coupling is weak and does not modify the structure; in this limit, the perturbation theory is applicable; therefore, Fermi's golden rule and the spectroscopic amplitudes characterize decay and reaction observables.

Let us demonstrate the approach using a well-known $^8\mathrm{Be} \to \alpha + \alpha$ example which, due to numerous previous theoretical studies [7,23,54,55], emerged as a benchmark for clustering methods. In addition, ^{8}Be is a stark example of collectivity and rotations in the continuum [3,56] where, as being well established experimentally in many light nuclei [6,8,9,57], strongly clustered rotational bands survive the complexity of many-body dynamics. In the limit where a channel is constructed from two α particles with structure limited to $\alpha[0]$, the norm kernel is diagonal and nonzero only when $2n + \ell \geq 4$ and ℓ is even; it can be computed analytically [58]:

$$\mathcal{N}^{(\ell)}_{nn'} = \delta_{nn'} 2(1 - 2^{2-2n-\ell}). \quad (7)$$

An example with four quanta in relative motion ($N_c = 2n + \ell$) is included in Table I. Result (7) highlights the bosonic nature of the α particle: Only even ℓ are allowed and with a growing number of quanta in the relative motion, $\mathcal{N}^{(\ell)}_{nn} \approx 2$.

In Fig. 1, we show the spectrum of the RGM Hamiltonian (5) computed using the SRG softened N3LO nucleon-nucleon interaction with a softening parameter $\lambda = 1.5$ fm^{-1} [59,60]. The results from the corresponding NCSM calculation $^8\mathrm{Be}[N_{\max} = 4]$ and the experimental spectrum are included for comparison. The radial part of the RGM wave function for different values of ℓ is shown in the inset. The channel states are limited to a maximum number of relative quanta $N_c \leq 12$. Tests with different Hamiltonians, with different values of $\hbar\Omega$, and with various truncations by oscillator quanta in the relative $\alpha - \alpha$ motion (N_c), as well as using more complex NCSM configurations for the α, indicate that this is a generic result. Additional details and comparisons can be inferred from the data in Table II.

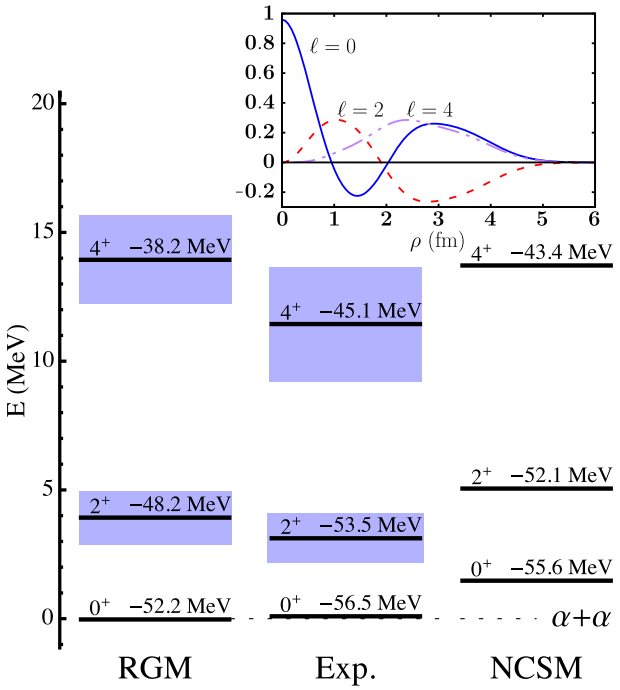

FIG. 1. Spectrum of RGM Hamiltonian with the SRG softened N3LO interaction ($\lambda = 1.5$ fm^{-1}) and $\hbar\Omega = 25$ MeV for a 2α system. Zero on the energy scale is set by the $\alpha + \alpha$ breakup threshold of the corresponding model. Levels are marked by spin and parity and by an absolute binding energy in units of MeV. The α binding energies for the $\alpha[0]$ and NCSM ($\alpha[4]$) calculations are −26.08 and −28.56 MeV, respectively. The inset shows the relative wave function of the two α clusters.

In comparison to the experiment, the relative energies and the rotational band states 0^+, 2^+, and 4^+ are well reproduced. The full no-core calculation, which in general includes cluster channels, naturally leads to a lower absolute binding energy, but our results suggest that these states in ^{8}Be are indeed nearly indistinct from $\alpha + \alpha$ RGM solutions. This structural information is highlighted by the large overlaps between parent states Ψ and RGM channels $\mathcal{F}_\ell$ shown in Table II.

For the example in Fig. 1, the validity of expansion (4) with $2n + \ell = N_c \leq 12$ is expected up to about $\rho \sim 4$ fm. Beyond that, the norm kernel transforms into that of

TABLE II. Select absolute values of spectroscopic amplitudes. Notation the same as those in Table I. Here, $N_c \leq 12$ for all models.

Parent	J^π	Channel	$\lvert\langle\Psi\rvert\mathcal{F}_\ell\rangle\rvert$
^{8}Be[4]	0^+	$\alpha[0]+\alpha[0]$	0.905
^{8}Be[4]	2^+	$\alpha[0]+\alpha[0]$	0.898
^{8}Be[4]	4^+	$\alpha[0]+\alpha[0]$	0.874
^{8}Be[4]	0^+	$\alpha[2]+\alpha[2]$	0.961
^{8}Be[4]	2^+	$\alpha[2]+\alpha[2]$	0.957
^{8}Be[4]	4^+	$\alpha[2]+\alpha[2]$	0.943
^{10}Be[4]	0^+	^{6}He[4] $+\alpha[0]$	0.820
^{10}Be[4]	2^+	^{6}He[4] $+\alpha[0]$	0.796
^{10}Be[4]	4^+	^{6}He[4] $+\alpha[0]$	0.638
^{12}C[4]	0^+_1	$\alpha[0]+\alpha[0]+\alpha[0]$	0.841
^{12}C[4]	0^+_2	$\alpha[0]+\alpha[0]+\alpha[0]$	0.229

independent particles, and, assuming that the resonance is narrow, we should match this to a wave function of two α particles with a relative motion described by an outgoing Coulomb wave. Our estimates for the width based on the standard techniques (see Refs. [33,61], and references therein) give 8.7 eV, 1.3 MeV, and 2.1 MeV for a channel radius $\rho_c = 3.6$ fm; the corresponding experimental widths are 5.6 eV, 1.5 MeV, and 3.5 MeV for the 0^+, 2^+, and 4^+ resonances, respectively. This value for ρ_c is selected to be in the middle of the area where our results are not sensitive to changes in the channel radius.

We utilize the same approach with the same parameters to examine the ground state cluster rotational band of ^{10}Be, also shown in Table II. The remarkable survival of rotations in the continuum displayed in this nucleus through clustering bands that persist despite the presence of weakly bound valence neutrons have been highlighted by recent experiments [57,62]. Our results reaffirm this phenomenon and open a path for its further theoretical investigation.

Finally, we discuss the 3α nature of bound and decaying states in ^{12}C. Various cluster geometries have been proposed for ^{12}C states [13,63,64], pointing to the major role α clustering plays in this nucleus and correspondingly for the formation of elements in nature. Here for the first excited 0^+ (Hoyle) state the fraction of the direct decay, currently believed to be less than 10% of the total, and its competition with the sequential, via ^{8}Be, one is of particular interest [65,66].

We employ the RGM procedure with three identical α particles, each in an $\alpha[0]$ configuration, with up to 12 quanta in relative motion and the same Hamiltonian as before. The results in Table II show the spectroscopic amplitudes for the ground state and for the first excited, 0^+_2 state, which could be a prototype of the Hoyle state.

The unconstrained RGM wave function defines initial amplitudes for all types of asymptotic three-α solutions. The amplitude for the sequential decay process, proceeding via the ground state of ^{8}Be, can be evaluated by constructing the constrained $^8\mathrm{Be}+\alpha$ channel separately and projecting it out. For the 0^+_2 state, the magnitude of the sequential decay amplitude is 89% of the total, with the remaining 11% corresponding to all other processes that do not proceed via the ^{8}Be ground state. These amplitudes, their interference, final state interactions, and phase space lead to observables; see Ref. [31] and references therein.

In summary, in this work we put forward a new approach that targets clustering reaction dynamics in light nuclei from *ab initio* principles. Our approach is based on the configuration interaction technique combined with the resonating group method, involves antisymmetrization over all nucleons, is translationally invariant, is applicable to various types of clustering, and under appropriate approximations reduces to well-established previously used techniques. Studies of ^{8}Be show the consistency of our results with other methods and good agreement with experimental data. We demonstrate the emergence and stability of the in-continuum rotational bands in beryllium isotopes. Starting from first principles, we conduct a triple-α clustering study of ^{12}C which is unbiased towards direct or sequential decay processes. As discussed throughout the text, we hope that our work will set an important milestone in the physics connecting structure and reactions. Further ongoing comparisons with experimental data, advanced numerical studies, studies of different Hamiltonians, and different approximations should provide an invaluable insight on the physics of clustering phenomena in atomic nuclei and quantum many-body systems, in general.

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