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Nuclear Structure with Discrete Non-Orthogonal Shell Model : new frontiers

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We present developments and applications for the diagonalization of shell-model hamiltonians in a discrete non-orthogonal basis (DNO-SM). The method, and its actual numerical implementation CARINA, based on mean-field and beyond-mean field techniques has already been applied in previous studies and is focused on basis states selection optimization. The method is benchmarked against a full set of *sd* shell exact diagonalizations, and is applied for the first time to the heavy deformed ²⁵⁴No nucleus.

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I. INTRODUCTION

In the recent decades, the advent of radioactive beam factories associated with developments of more sophisticated experimental methods has enabled to discover new manifestations of many-body nuclear dynamics in many places of the nuclear chart. New phenomena like halo systems, two-proton radioactivity, occurrence of new magic numbers, vanishing of shell closures, soft dipole modes, or even searches for superheavy nuclei have been observed and have stimulated the continuous developments and improvements of theoretical methods in order to interpret such phenomena.

Among the various theoretical frameworks available, the Shell-Model (SM) or Configuration Interaction (CI), either in its no-core or valence space implementations, has always been one of the most powerful methods in the description of quantum nuclear systems [1, 2], in particular with the numerical development of efficient diagonalization codes which have opened the era of the so-called "Large Scale Shell-Model calculations" for light and medium-mass nuclei up to $A \sim 150$ [3–8] and have become the method of choice to explain the observed nuclear phenomena, guide experimental programs, and not the least, allowed for a deeper understanding of many astrophysical objects and processes in which exotic nuclei often play the key role. But its success was always mirrored by the exponential growth of the systems basis involved. It is also true that variational methods with symmetry breaking and restoration have also shown great success for decades and have proven to a certain extent to be applicable over the nuclear chart from the lightest nuclear systems to the most heavy ones [9–11].

Although, these methods provide distinct description, the merging of the mean-field techniques within the shell-model formalism has already been developed used in the literature in the past, starting from the pioneering work of Ripka [12], later followed by the different Vampir implementations [13, 14]. One of the major achievements up to now was proposed by the Tokyo group with the Monte Carlo Shell-Model [15–17]. And more recently several implementations were used, either in an isolate manner [18, 19] or in a more ambitious scale with the

recent development of the Taurus numerical suite [20, 21]. In the present work, we present formalism of the Discrete Non-Orthogonal Shell-Model (DNO-SM) and its associated numerical implementation Carina. The DNO-SM amounts to diagonalize valence shell-model hamiltonians in a non-orthogonal basis with the use of beyond-mean-field techniques. The detailed framework is exposed in the next section and applications to *sd* shell nuclei in comparison with exact diagonalizations are discussed in section III. The final section exposes an application a very heavy system in the ²⁵⁴No case.

II. THEORETICAL FRAMEWORK

A. Shell Model formulation revisited

1. The diagonalization dilemma

The ultimate question in the Shell Model, once a physically meaningful valence space \mathcal{E} is equipped together with the associated effective interaction $\hat{\mathcal{V}}$ for the problem at hand, is to tackle the secular equation

$$\hat{\mathcal{H}}|\Psi\rangle = E|\Psi\rangle \quad (1)$$

where $\hat{\mathcal{H}}$ represents the effective Hamiltonian composed of $\hat{\mathcal{V}}$ and a one-body single-particle energy $\{e_i\}$ part

$$\hat{\mathcal{H}} = \sum_{i \in \mathcal{E}} e_i a_i^\dagger a_i + \frac{1}{4} \sum_{ijkl \in \mathcal{E}} \langle ij|\hat{\mathcal{V}}|kl\rangle a_i^\dagger a_j^\dagger a_l a_k. \quad (2)$$

$\{a_i^\dagger\}$ and $\{a_i\}$ are creation and annihilation operators satisfying the common anti-commutation rules for fermionic systems.

By defining a set of basis states $\mathcal{B} = \{|\phi_m\rangle, m \in \mathbb{N}\}$ constructed from the single-particle spherical oscillator valence space \mathcal{E} with which we can write the eigenstate $|\Psi\rangle$ as

$$|\Psi\rangle = \sum_{m=1}^{\dim(\mathcal{B})} c_m |\phi_m\rangle, \quad (3)$$

the classic Shell Model resolution of (1) then amounts to addressing the eigenvalue problem

$$\sum_{m=1}^{\dim(\mathcal{B})} \mathcal{H}_{m'm} c_m = E c_{m'} \quad (4)$$

by an exact diagonalization of the Hamiltonian matrix $\mathcal{H}_{m'm} = \langle \phi_{m'} | \hat{\mathcal{H}} | \phi_m \rangle$ in the model space $\mathcal{H} = \overline{\text{Span } \mathcal{B}}$. The dimensionality of \mathcal{B} represents the huge technical challenge of the Shell Model, as well known in the literature once far away from closed shells. To deal with this dilemma, we look for a replacement of \mathcal{B} with a different family of basis states. The existence of such basis takes the root in the original idea of the Generator Coordinate Method (GCM). As we shall discuss in the following, it can be however viewed in an independent status with respect to the GCM, thanks to the work of the authors in Ref. [22].

2. Discrete non-orthogonal basis

The starting point of the GCM is the hypothesis that one can find a family of states depending on the continuous (generator) coordinate(s) q

$$\Gamma = \{ |\Phi(q)\rangle \mid q \in \mathbb{R} \} \quad (5)$$

so that the latter forms a model subspace $\mathcal{H}_q = \overline{\text{span } \Gamma} \subseteq \mathcal{H}$ following the nature of the coordinate(s) q that we choose in the generation of Γ . The core of our presentation of \mathcal{H}_q relies on the following existence theorem first noticed in Ref. [22]. Suppose \mathcal{H}_q is a separable Hilbert subspace, i.e. $\mathcal{H}_q \subseteq \mathcal{H} \subset \mathcal{L}^2$ where \mathcal{L}^2 denotes the full Hilbert space associated with the space of square integrable functions, the separability property of \mathcal{H}_q implies the existence of a countable family

$$\Gamma_0 = \{ |\Phi(q_i)\rangle \mid i \in \mathbb{N} \} \subset \Gamma \quad (6)$$

which is in general skew or non-orthogonal set of states with the property $\mathcal{H}_q = \overline{\text{span } \Gamma_0}$. This enables us to tackle now the diagonalization of $\hat{\mathcal{H}}$ in the subspace \mathcal{H}_q represented by the discrete non-orthogonal basis set Γ_0 . Indeed, by expressing the eigenstate $|\Psi\rangle$ as

$$|\Psi\rangle = \sum_{i=0}^{\infty} f(q_i) |\Phi(q_i)\rangle, \quad (7)$$

the projection of (1) in \mathcal{H}_q becomes equivalent to the generalized eigenvalue problem

$$\sum_{i=0}^{\infty} \left[\mathcal{H}(q_{i'}, q_i) - E \mathcal{N}(q_{i'}, q_i) \right] f(q_i) = 0 \quad (8)$$

where $\mathcal{O}(q_{i'}, q_i) = \langle \Phi(q_{i'}) | \hat{\mathcal{O}} | \Phi(q_i) \rangle$ ($\hat{\mathcal{O}} = \hat{\mathcal{H}}, \mathcal{K}$) are the Hamiltonian and norm matrix elements and $f(q_i)$ the expansion coefficient.

Therefore, instead of using the basis \mathcal{B} spanning the full model space \mathcal{H} , the above presented theorem on the existence (not necessarily unique) of a discrete non-orthogonal basis set of $\hat{\mathcal{H}}$ suggests that :

1. the diagonalization of $\hat{\mathcal{H}}$ in \mathcal{H}_q becomes “exact” when $\mathcal{H}_q = \mathcal{H}$, which means the coordinate(s) q must be chosen so as to “exhaust” in some way the space \mathcal{E} ;
2. the truncation of the infinite countable set Γ_0 could be done in a variational way such that the finite sum

$$|\Psi\rangle \approx \sum_{i=0}^n f(q_i) |\Phi(q_i)\rangle \quad (9)$$

yields an optimal approximation.

Whether we are able to choose q to fulfil the condition $\mathcal{H}_q = \mathcal{H}$ can be verified a posteriori. What needed is then an efficient truncation method of Γ_0 , which we shall address now.

3. Truncation method with Caurier’s minimization technique

The existence theorem as presented previously has enabled us to transform the classic Shell Model eigenvalue problem (4), formulated in the orthonormal basis \mathcal{B} , into the generalized one (8) through the discrete non-orthogonal basis Γ_0 . As noted earlier by the authors of Ref. [22], the minimization technique originally proposed by E. Caurier in Ref. [23] provides an iterative prescription to truncate Γ_0 in a variational way.

It proceeds as follows, in Caurier’s words [23] : “the first point q_0 is the one such that $|\Phi(q_0)\rangle$ minimizes the energy. The second point q_1 is chosen in such a way that the energy obtained from diagonalizing the Hamiltonian in the 2–dimensional space spanned by $|\Phi(q_0)\rangle$ and $|\Phi(q_1)\rangle$ be a minimum. One proceeds in the same way to determine the third basis vector $|\Phi(q_2)\rangle$ etc...”.

The technique was however implemented only in toy model examples of Hydrogen atom in molecular physics (cf. e.g. [24]) and has never been considered in realistic nuclear structure calculations. Therefore, instead of the conventional problem represented by $(\hat{\mathcal{H}}, \mathcal{H}, \mathcal{B})$, our current work exploits fully this technique for the first time in the Shell Model framework formulated in terms of $(\hat{\mathcal{H}}, \mathcal{H}_q, \Gamma_0)$. This resulting model will be from now on referred to as *Discrete Non-Orthogonal Shell Model* (DNO-SM).

To be now more precise in the practical realization of the DNO-SM, we assume that the Projected Constrained Hartree–Fock (PCHF) approach provides us with a basis generation method which will be our focus in the next subsection. However, before going further, let us note that, the Caurier’s original technique allows to minimize one state at a time. In practice, we find that to cover different cases, it is more preferable to obtain various excited states by a single minimization. Hence, the

generalization of Caurier's technique to deal with the minimization of many states simultaneously will be shown later.

B. Projected constrained Hartree-Fock basis

Having introduced the general framework of our approach to the dimensionality problem encountered in the classic Shell Model, we present now the construction of the many-body basis in the DNO-SM. The choice of degrees of freedom here is important to take into account correlations as much as possible in the generation of the basis. This should be inferred on physical grounds. Moreover, the many-body basis must conserve important symmetries of the effective Hamiltonian, in particular, the cases associated with conserved quantities such as the angular momentum and particle numbers. Such basis could be built upon the Constrained Hartree-Fock (CHF) method which relies on the rotational symmetry breaking at the mean-field to incorporate deformations. A projection on good angular momentum is required later before proceeding to the full diagonalization.

A Hartree-Fock (HF) state $|\Phi(q)\rangle = \prod_{i=1}^A a_i^\dagger |0\rangle$ for a nucleus of A -particles is obtained from CHF calculations under the conditions

$$\langle \Phi | \hat{Q}_{\lambda\mu} | \Phi \rangle = Q_{\lambda\mu}, \quad \langle \Phi | \hat{J}_m | \Phi \rangle = \langle \hat{J}_m \rangle \quad (m = x, z), \quad (10)$$

where $\hat{Q}_{\lambda\mu} = r^\lambda Y_{\lambda\mu}(\theta, \varphi)$ is the multipole operator expressed in terms of spherical harmonics $Y_{\lambda\mu}$ and \hat{J}_m the components of the total angular momentum operator $\hat{\mathbf{J}}$. Here $Q_{\lambda\mu}$ and $\langle \hat{J}_m \rangle$ are constraining expectation values that we fix before the calculation. Once this is done, the resulting HF state is projected onto good angular momentum J through the usual procedure using the operator

$$\mathcal{P}_{MK}^J(A) = \frac{2J+1}{4\pi^2(3-(-)^A)} \times \int_0^{2\pi} d\alpha \int_0^\pi d\beta \int_0^{\gamma_{\max}} d\gamma \mathcal{D}_{MK}^{J*}(\alpha, \beta, \gamma) \hat{R}(\alpha, \beta, \gamma), \quad (11)$$

where $\gamma_{\max} = (3-(-)^A)\pi$, $\hat{R}(\alpha, \beta, \gamma)$ and $\mathcal{D}_{MK}^{J*}(\alpha, \beta, \gamma)$ denote the rotation operator and the Wigner matrix. This provides us a family of PCHF states characterized by the angular momentum projection onto the intrinsic axis $|K| \leq J$ and the coordinate q for a given J

$$\Gamma = \{\mathcal{P}_{MK}^J(A)|\Phi(q)\rangle \mid q \in \mathbb{R}\} \quad (12)$$

with which we can now formulate the DNO-SM's working equations. This procedure to generate the DNO-SM basis is implemented to treat both odd- and even-nuclei without further assumptions. More specifically, we do not impose any self-consistent symmetries (e.g. no time-reversal, no parity conservation) at the HF mean field

to exploit at best what is offered by the single-particle valence space \mathcal{E} . The construction of DNO-SM basis for odd nuclei is done via the constrain of angular momentum components \hat{J}_m ($m = x, z$) which, as we will show later, can provide a very good many-body basis for such nuclei. Since there is no self-consistent symmetries adopted here, the angular momentum projection demands to perform integrations over Euler angles $\Omega = (\alpha, \beta, \gamma)$ in full intervals without restrictions. To do so, we have developed an analytical formula that performs an exact integration over (α, γ) whose derivation is presented in Annexe B. The integration over β is done numerically using the Gauss-Legendre quadrature rule.

C. DNO-SM formalism

1. Secular equation in non-orthogonal PCHF basis

Let us start with the ansatz (7) where we specify the eigenstate of $\hat{\mathcal{H}}$ by $|\alpha JM\rangle$ of good total angular momentum J , its projection M in the laboratory frame and an index α labelling indices of corresponding energy levels and other quantum numbers. In terms of the PCHF states $\mathcal{P}_{MK}^J|\Phi(q)\rangle \in \Gamma_0 \subset \Gamma$, it is given by

$$|\alpha JM\rangle = \sum_{q,K} f_\alpha^{(J)}(q; K) \mathcal{P}_{MK}^J|\Phi(q)\rangle. \quad (13)$$

To simplify the notation, we omit the dependence on mass number A in the projection operator \mathcal{P}_{MK}^J and q is understood to take discrete values. The projected equation (8) then becomes

$$\sum_{q,K} \left[\mathcal{H}_{K'K}^J(q', q) - E_\alpha^{(J)} \mathcal{N}_{K'K}^J(q', q) \right] f_\alpha^{(J)}(q; K) = 0 \quad (14)$$

where the Hamiltonian and the norm matrix elements $\mathcal{O}_{K'K}^{(J)}(q', q) = \langle \Phi(q') | \hat{\mathcal{O}} \mathcal{P}_{K'K}^J | \Phi(q) \rangle$ (with $\hat{\mathcal{O}} = \hat{\mathcal{H}}, \mathcal{N}$) are evaluated through a three-fold integration over Euler angles $\Omega = (\alpha, \beta, \gamma)$

$$\mathcal{O}_{K'K}^{(J)}(q', q) = \frac{2J+1}{4\pi^2(3-(-)^A)} \times \int d\Omega \mathcal{D}_{MK}^{J*}(\Omega) \langle \Phi(q') | \hat{\mathcal{O}} \hat{R}(\Omega) | \Phi(q) \rangle. \quad (15)$$

The general formula of this matrix element for a two-body operator respecting the rotational symmetry is presented in Annexe A.

The treatment of the generalized eigenvalue problem (14) has been well documented in the framework of the generator coordinate method. We follow the standard technique that begins with the determination of the natural eigenbasis functions $u_i^{(J)}(q; K)$ of the norm matrix

$$\sum_{q,K} \mathcal{N}_{K'K}^J(q', q) u_i^{(J)}(q; K) = \eta_i^{(J)} u_i^{(J)}(q'; K'). \quad (16)$$

By retaining only positive norm eigenvalues that we denote by $\{\eta_i^{(J)} > 0, i \in \mathbb{N}\}$, the so-called natural state characterized by the corresponding norm eigenvalue $\eta_i^{(J)}$ is defined as

$$|\eta_i^{(JM)}\rangle = \frac{1}{\sqrt{\eta_i^{(J)}}} \sum_{q,K} u_i^{(J)}(q; K) \mathcal{P}_{MK}^J |\Phi(q)\rangle, \quad (17)$$

$$\langle \eta_{i'}^{(JM)} | \eta_i^{(JM)} \rangle = \delta_{i'i}$$

and satisfies the orthogonality condition. This natural basis allows to transform the projected equation in the non-orthogonal PCHF basis onto the usual eigenvalue value problem of the form

$$\sum_{i'} \mathcal{H}_{i'i}^{(J)} g_{i'}^{(J)} = E_\alpha^{(J)} g_i^{(J)} \quad (18)$$

where the Hamiltonian matrix now is expressed between orthogonal natural basis states $\{|\eta_i^{(JM)}\rangle\}$

$$\mathcal{H}_{i'i}^{(J)} = \frac{1}{\sqrt{\eta_{i'}^{(J)} \eta_i^{(J)}}} \sum_{q',K',qK} u_{i'}^{(J)*}(q'; K') \times \mathcal{H}_{K'K}^J(q', q) u_i^{(J)}(q; K). \quad (19)$$

The nuclear state $|\alpha JM\rangle$ is thus a linear superposition in the natural basis

$$|\alpha JM\rangle = \sum_i g_i^{(J)} |\eta_i^{(JM)}\rangle \quad (20)$$

with the transformation onto the non-orthogonal PCHF basis expressed through the expansion coefficient $f_\alpha^{(J)}(q; K)$ of (13)

$$f_\alpha^{(J)}(q; K) = \sum_i \frac{g_i^{(J)}}{\sqrt{\eta_i^{(J)}}} u_i^{(J)}(q; K). \quad (21)$$

One can notice that $f_\alpha^{(J)}(q; K)$ is not properly normalized and does not represent the probability amplitude of finding a given configuration of Γ_0 . To be able to analyze the content of the nuclear states, we can define the normalized probability amplitude to find a component $\mathcal{P}_{MK}^J |\Phi(q)\rangle$ in the state $|\alpha JM\rangle$ by

$$\mathcal{M}_\alpha^{(J)}(q; K) = \sum_{q',K'} [\hat{N}^{1/2}]_{K'K}^{(J)} f_\alpha^{(J)}(q'; K'). \quad (22)$$

The corresponding probability to find the intrinsic angular momentum component K or the component q in the state $|\alpha JM\rangle$ is respectively given by

$$\mathcal{P}_\alpha^{(J)}(K) = \sum_q \left| \mathcal{M}_\alpha^{(J)}(q; K) \right|^2, \quad (23)$$

$$\mathcal{P}_\alpha^{(J)}(q) = \sum_K \left| \mathcal{M}_\alpha^{(J)}(q; K) \right|^2,$$

with the normalization relation

$$\sum_K \mathcal{P}_\alpha^{(J)}(K) = \sum_q \mathcal{P}_\alpha^{(J)}(q) = 1. \quad (24)$$

2. Truncation of the PCHF basis with the generalized minimization technique

We come now to the truncation of the discrete family Γ_0 with the minimization technique. The original idea of E. Caurier about how to choose states of Γ_0 is quite straightforward. That is, applying to the present case including the angular momentum projection, based on the selection of discrete values of the coordinate q which minimizes the energy, i.e. we let the Hamiltonian itself to choose what is the best state from a variational viewpoint. It is implicitly understood, in Caurier's paper, that it is the ground state or some first excited state which must be chosen beforehand. Then the following iterative procedure can be implemented :

- 1) Fix the state $E_\alpha^{(J)}$ to be minimized with α indexing energy levels ;
- 2) Define a searching region of the coordinate(s) q ;
- 3) Start from the first point which can be chosen as the HF minimum ;
- 4) Solve the projected Shell Model circular equation (14) over the whole searching region of q to find the second state and proceed the same way in next iterations until the convergence of $E_\alpha^{(J)}$.

In practice, we observe that fixing (α, J) will exclude in the minimization the states of Γ_0 which could be relevant for an other state (α', J') . Hence, small components of the wave functions could be missed whereas the overall spectrum remains well described. The key point is thus, minimizing as many excited states at the same time as possible will eventually lead to the improvement of one and another mutually and also the ground state. This idea leads us to generalize the above iterative procedure in the following way : one lets the Hamiltonian to choose not only the coordinate(s) q but also *to determine which state (α, J) one should minimize*. The determination of (α, J) is done by taking the basis state of Γ_0 that minimizes it the most among all states that one wants to describe.

The minimization procedure as such requires an organizational scheme of partitioning the coordinate(s) q , which form in general a multi-dimensional surface. Although it is possible to determine all of them simultaneously in principle, it might not be necessary to do so. The reason is that, as a consequence of the existence theorem, different countable sets $\Gamma_0 \subset \Gamma$ could be qualified as basis for \mathcal{H}_q . In practice, we define the following organization of the coordinate(s) q with different levels of varying them. The role of deformation parameters $Q_{\lambda\mu}$ and of the constrained angular momentum $\langle \hat{J}_m \rangle$, $m = x, z$ is kept distinguished. While the former is let varied and determined by the Hamiltonian itself using the minimization technique, the latter is fixed in advance. That is, we let the minimization exhaust the multi-dimensional deformation surface $Q_{\lambda\mu}$ at $\langle \hat{J}_m \rangle = J_m^{(1)}, J_m^{(2)}, J_m^{(3)}, \dots$, where $\{J_m^{(i)}\}$ here are actual constraining values from input.

3. Choice of the coordinate(s) q

In order to generate I_0 , in this present work, we limit ourselves to quadrupole deformations (axial and triaxial) as the generator coordinates, whose expectation values in a HF state $|\Phi\rangle$ are denoted by Q_{20}, Q_{22} respectively

$$Q_{20} = \sqrt{\frac{16\pi}{5}} \sum_{\tau=p,n} \langle \Phi | \hat{Q}_{20}^{(\tau)} | \Phi \rangle \quad (25)$$

$$Q_{22} = \sqrt{\frac{16\pi}{5}} \sum_{\tau=p,n} \langle \Phi | (\hat{Q}_{2-2}^{(\tau)} + \hat{Q}_{22}^{(\tau)}) | \Phi \rangle. \quad (26)$$

In this particular case, we use the usual Hill-Wheeler (β, γ) parameters which are related to (Q_{20}, Q_{22}) through the total quadrupole moment $Q = \sqrt{Q_{20}^2 + Q_{22}^2}$

$$\beta = \frac{b^2 Q \sqrt{5\pi}}{3r_0^2 A^{5/3}}, \quad \gamma = \arctan\left(\frac{Q_{22}}{Q_{20}}\right) \quad (27)$$

where b^2 (in fm²) is the harmonics oscillator parameter

$$b^2 = \frac{41.4}{45A^{-1/3} - 25A^{-2/3}}, \quad (28)$$

and A and $r_0 = 1.2$ (in fm) are the nuclear mass number and radius parameter.

Within the shell-model formalism, the use of valence spaces and truncation of the Hilbert space implies the need of effective hamiltonians as well as effective operators. Effective operators can be derived by Many-Body Perturbation Theory [26] but quadrupole operators are usually renormalized with the use of an effective charge. The effective charge have been defined by several authors, we use here the notation defined in ref [27] :

$$e_{eff}^p = (1 + \chi)e, \quad e_{eff}^n = \chi e \quad (29)$$

with χ being the electric polarization charge. χ value is intimately connected to the valence space used and can be derived by Many-Body Perturbation Theory [26] and is shell dependent but for $0\hbar\omega$ spaces, the microscopic Dufour-Zuker [28] $\chi_p = 0.31$, $\chi_n = 0.46$ are standard values. Finally, for mass quadrupole operators, we will use

$$e_{eff}^p = e_{eff}^n = (1 + \chi_p + \chi_n)e$$

to be consistent with the deformation parameters defined above.

III. BENCHMARK AND COMPARISON IN SD NUCLEI

A. Even nuclei

To assess the quality of the PCHF basis I_0 against the oscillator one in the classic Shell Model, we perform a

systematic comparison of two models in even sd nuclei using the USDB effective interaction [29]. This comparison is shown in Table II, where we calculate and compare the ground state and the first excited states $2_1^+, 4_1^+$ energies as well as the corresponding $E2$ -transition probabilities for Neon, Magnesium, Silicon and Argon even-even isotopes. To give more details of these calculations, we use the same set of states $J_\alpha \in \{0_1, 2_{1,2}, 4_1, 8_1, 12_1, 16_1\}$ whenever possible. After a first minimization to find non- cranked CHF states over the range $\gamma \in [0^\circ, 60^\circ]$ discretized into a one-dimensional mesh of N_g points, the diagonalization is then iterated with consecutive constrained values $\langle \hat{J}_z \rangle = -2, -4, -8, -12, -16$. The discretization in the β -direction is given in Table I together with the HF minimum point $(\beta_{\min}, \gamma_{\min})$ for each nucleus. Angular Momentum Projection is performed for all these calculations using the same number of points, namely, 11 points for the analytical integration over the angles $\alpha, \gamma \in [0, 2\pi]$ and 20 Gauss-Legendre quadrature points for the integration over the angle $\beta \in [0, \pi]$. As we can see in Table II, the agreement between two models is excellent for both relative energies and $E2$ -transition probabilities, indicating that the wave functions have already converged for the considered states. We observe however a small difference of order $\sim 0.1 - 1.0$ MeV in the ground state binding energy with respect to the exact result, which tends to become larger in nuclei at mid-shell than in others. This is potentially due to the fact that our minimization technique builds up the many-body basis based on a finite set of states preliminarily defined, in the present case, i.e. the set $J_\alpha \in \{0_1, 2_{1,2}, 4_1, 8_1, 12_1, 16_1\}$, hence, indirectly omits basis states relevant for other states not included in the set. Therefore, the representation of the effective Hamiltonian in the truncated basis I_0 is not fully complete as the construction is under way. This is in contrast to the full SM diagonalization in the oscillator basis because all many-body matrix elements of the effective Hamiltonian are available once the valence space is defined.

TABLE I: Discretization of the (β, γ) plane for minimization procedure for selected sd nuclei using the USDB effective interaction.

β	N_b	N_g	nucleus	β_{\min}	γ_{\min}
[0.1, 0.8]	11	9	^{20}Ne	0.6	0.0
			^{22}Ne	0.56	0.0
[0.1, 0.6]	11	9	^{24}Ne	0.35	23.8
			^{26}Ne	0.28	0.0
[0.1, 0.54]	7	9	^{28}Ne	0.22	0.0
			^{24}Mg	0.50	12.0
			^{26}Mg	0.45	34.0
			^{28}Mg	0.37	0.0
			^{30}Mg	0.24	0.0
			^{28}Si	0.42	60.0
			^{30}Si	0.32	46.8
			^{32}Si	0.25	60.0
			^{32}S	0.0	–
			^{34}S	0.17	60.0
			^{36}Ar	0.2	60.0

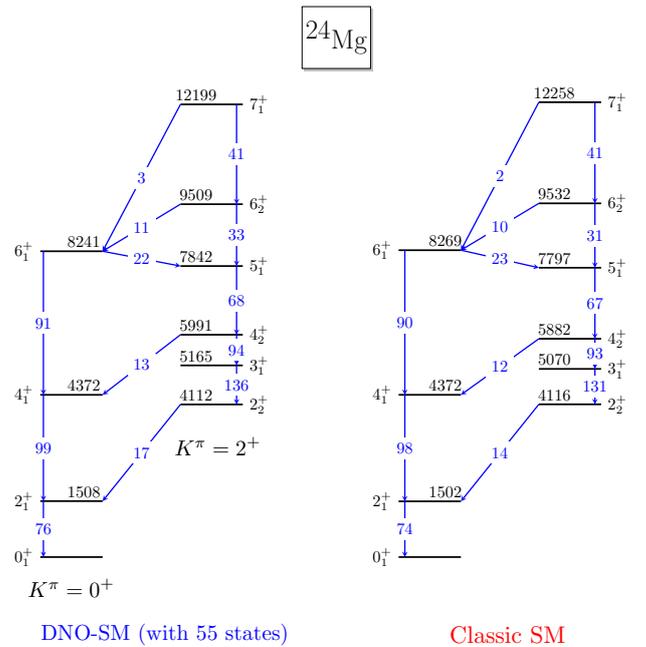


FIGURE 1: ^{24}Mg spectrum calculated with the USDB interaction using the DNO-SM compared to the classic SM diagonalization. Black numbers are relative energies (in keV) and blue ones the $B(E2)$ values (in $e^2 \cdot \text{fm}^4$). K denotes the dominant wave-function component of different members of the band.

We concentrate now on a more detailed analysis of a typical example of deformed nuclei in the sd shell with the DNO-SM : ^{24}Mg . This nucleus was extensively studied in the past within various approaches. It is well established that it has a triaxial shape in its ground state with a rotational band built on top. Moreover, the triaxiality manifests itself in the existence of the so-called γ -band that was experimentally observed. In Figure 1, we show the DNO-SM calculation of these two bands using the USDB effective interaction in comparison with the classic SM result. The minimization technique optimizes states of both bands simultaneously with the same discretization of (β, γ) given in Table I. Cranked CHF states are added in the same manner as the previous comparison. We find an excellent agreement for relative energies and transition properties in the DNO-SM calculation with 55 states compared to the SM result. The ground state binding energy is found in this calculation to be -86.86 MeV versus the exact one -87.10 MeV.

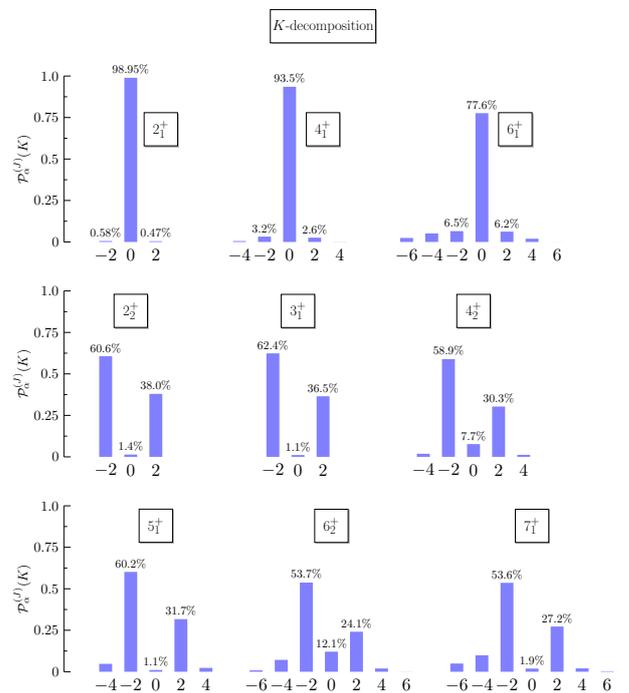


FIGURE 2: Decomposition of states into K -contribution in ^{24}Mg

Figure 2 presents the wave function content of each

TABLE II: Systematics comparison of the diagonalization in the model spaces \mathcal{H}_q and \mathcal{H} of the Shell Model in even sd nuclei. The absolute ground state energy E_{gs} and relative energies of the first 2^+ and 4^+ are given in MeV. Their reduced transition probabilities $B(E2; 2_1^+ \rightarrow 0_1^+)$ and $B(E2; 4_1^+ \rightarrow 2_1^+)$ are in $\text{e}^2 \cdot \text{fm}^4$ unit. N_q denotes the number of CHF states $|\Phi(q)\rangle$ found with the minimization procedure.

nucleus	\mathcal{H}_q			\mathcal{H}		E_{gs} (MeV)		$B(E2; 2_1^+ \rightarrow 0_1^+)$		$B(E2; 4_1^+ \rightarrow 2_1^+)$	
	N_q	2_1^+	4_1^+	2_1^+	4_1^+	\mathcal{H}_q	\mathcal{H}	\mathcal{H}_q	\mathcal{H}	\mathcal{H}_q	\mathcal{H}
^{20}Ne	16	1.76	4.14	1.75	4.18	-40.40	-40.47	47.0	46.9	56.3	55.3
^{22}Ne	41	1.37	3.39	1.36	3.36	-57.32	-57.58	48.1	46.9	64.0	63.3
^{24}Ne	39	2.13	4.01	2.11	3.99	-71.26	-71.72	38.8	38.7	31.9	31.3
^{26}Ne	26	2.12	3.72	2.06	3.51	-80.98	-81.56	39.6	38.5	37.8	33.8
^{28}Ne	12	1.55	2.82	1.62	2.99	-86.13	-86.54	34.3	34.1	32.7	30.7
^{24}Mg	42	1.52	4.37	1.50	4.37	-86.82	-87.10	76.1	74.4	99.1	97.5
^{26}Mg	50	1.80	4.36	1.89	4.36	-104.56	-105.52	66.1	65.2	27.5	18.0
^{28}Mg	50	1.40	4.07	1.52	4.17	-119.71	-120.50	62.9	60.2	75.7	67.5
^{30}Mg	21	1.50	3.89	1.59	3.89	-129.77	-130.47	53.0	49.1	39.6	32.5
^{28}Si	71	2.12	4.78	1.93	4.61	-135.54	-135.86	77.4	77.9	106.8	109.6
^{30}Si	46	2.25	5.59	2.26	5.33	-154.09	-154.75	46.9	45.9	54.0	15.8
^{32}Si	43	1.99	5.79	2.05	5.88	-170.06	-170.52	41.1	42.5	66.9	65.2
^{32}S	50	2.05	4.55	2.16	4.65	-182.10	-182.45	48.0	46.9	69.2	66.8
^{34}S	36	2.01	4.66	2.13	4.83	-202.08	-202.50	38.3	36.0	51.7	48.0
^{36}Ar	12	1.81	4.46	1.82	4.49	-230.22	-230.28	50.4	50.6	63.2	62.9

member of two bands in terms of the intrinsic angular momentum contributions, the K quantum number. The small K -mixing via the $K = 0, 2$ components reflects the weak interband transitions observed in the $B(E2)$ values. This confirms in a microscopic calculation the existence of the γ -band known from geometrical models in ^{24}Mg , which is expected given the validity of the USDB interaction in this mass region.

B. Odd nuclei

The above systematic benchmark has shown our DNO-SM's efficiency compared to the classic SM in even nuclei. As previously mentioned, the present framework is also capable to deal with odd nuclei in the same way without further treatments of the odd particle at the Hartree-Fock level. We find that the cranking Hartree-Fock can provide an excellent approach to set up the initial set of PCHF states from which we construct the basis Γ_0 through the diagonalization-minimization process. To illustrate this, we present a DNO-SM calculation of ^{25}Mg whose spectrum appears in Figure 3 compared to the classic SM one. This nucleus is known to have for instance two distinct bands : the ground state band of $K = 5/2$ and an excited band of $K = 1/2$. Employing the USDB effective interaction, this assignment is clearly seen in the wave function structure of each member of the bands as shown in Figure 4. The minimization is car-

ried out with a discretization of 7 points $\beta \in [0.1, 0.51]$, 8 points $\gamma \in [1.5^\circ, 60^\circ]$ and with cranking components $\langle \hat{J}_z \rangle = -1/2, -3/2, -5/2, -7/2, -9/2$. The spectrum of two bands is reproduced remarkably well with a rms error of 44 keV, using 61 CHF states. The ground state binding energy is found to be -93.89 MeV versus -94.40 MeV in the exact SM result.

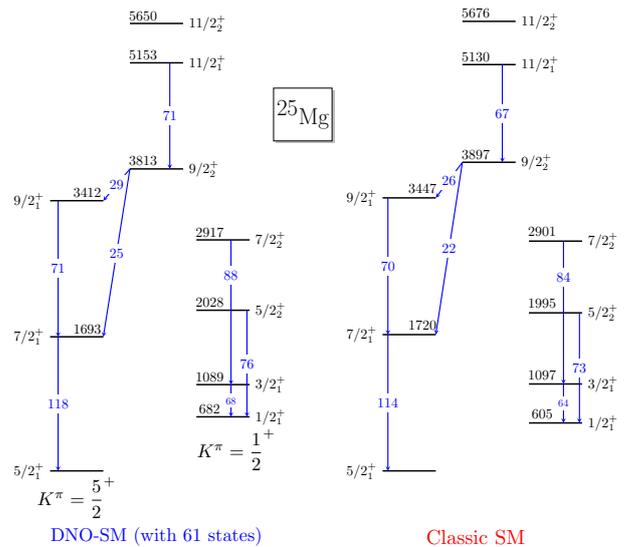


FIGURE 3: ^{25}Mg spectrum

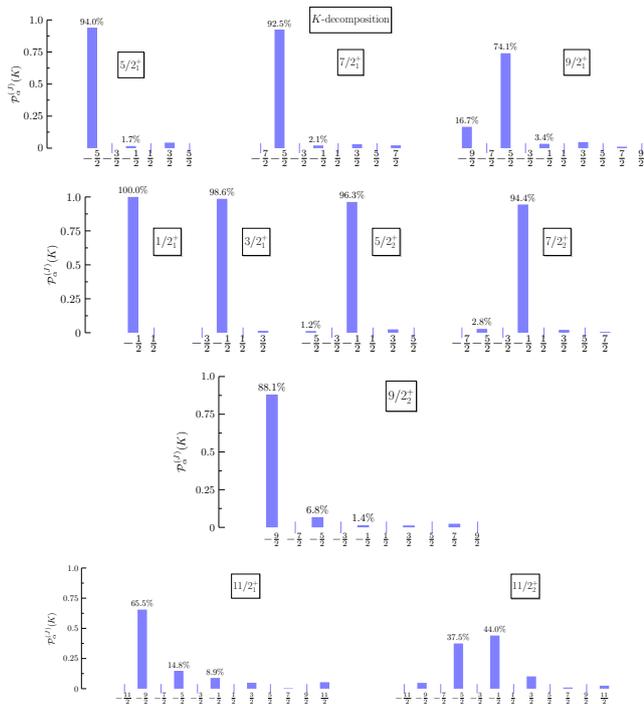


FIGURE 4: Decomposition of states into K -contribution in ^{25}Mg

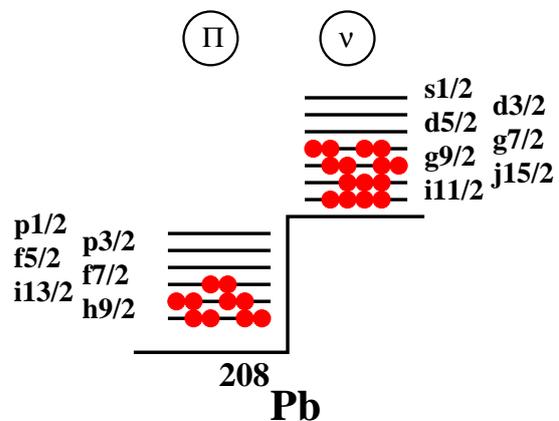


FIGURE 5: Valence space above ^{208}Pb

IV. A FIRST SHELL MODEL CALCULATION OF ^{254}No

The quest for superheavy elements is a subject under intensive experimental investigations and usually, the predictions for the shell stabilization of the superheavy elements predictions rely essentially on "standard" mean-field calculations. In the following, we will apply the DNO-SM method to illustrate its applicability in the context of superheavy systems and we propose here for the first time, a shell-model type of description of ^{254}No superheavy nucleus, using the DNO-SM. The shell-model valence space is spanned by the full $Z=82-126$ proton major shell and the full $N=126-184$ neutron major shell beyond ^{208}Pb , namely, the single proton orbitals $0h_{9/2}$, $1f_{7/2}$, $0i_{13/2}$, $1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$, and the single neutron orbitals $1g_{9/2}$, $0i_{11/2}$, $0j_{15/2}$, $2d_{5/2}$, $3s_{1/2}$, $1g_{7/2}$, $2d_{3/2}$ (the valence space is illustrated in in Fig. 5). As effective interaction, we use the modified Kuo-Herling realistic interaction (see [31] for details) which was applied with great success along the $N=126$ isotones [30, 31]. The single particle energies are borrowed from ^{209}Bi and ^{209}Pb spectra for protons and neutrons respectively.

^{254}No is a deformed nucleus whose spectroscopy has been intensively investigated the recent years. In addition to the observation of its rotational Yrast structure, a side $K = 3+$ band and two long lived isomers have been observed [32, 33]. Figure 6 shows the potential energy surface obtained for the mass (β, γ) deformation parameters (obtained from the mass quadrupole moments defined in section II C 3. The deformation landscape shows a clear prolate axial minimum around $\beta \sim 0.2$ extending moderately towards non-axial shapes.

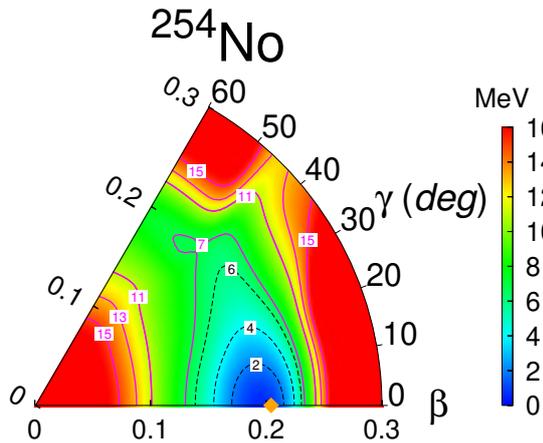


FIGURE 6: Potential Energy Surface (PES) of ^{254}No calculated with the Kuo-Herling effective interaction where the yellow diamond is the axial HF minimum with the mass quadrupole parameter $\beta = 0.2$.

All the considered states are calculated with the minimization technique over a restricted region around the corresponding HF minimum. The spectrum of ^{254}No resulting from these calculations is shown in figure 7 as the function of the number of HF states retained by the minimization procedure. With a relatively small number of basis states, we observe a fast and good convergence of the low-lying members of the Yrast band but also for the higher lying isomer 8^- isomer. As already shown in the previous section, the DNO-SM allows analysis of the states under study in terms of intrinsic quantities, namely, deformations (β, γ) and the intrinsic angular momentum. The whole low-lying spectrum is presented in figure 8. The various states are shown and grouped in 3 structures : a $K = 0^+$ Yrast rotational band, a $K^\pi = 3^+$ multiplet and the $K^\pi = 8^-$ state. There is an excellent agreement for the reproduction of the Yrast rotational sequence, and the 8^- isomeric state. The 3^- state band-head of the $K = 3$ multiplet is lying a little bit too low, by the interband spacing is also very well reproduced. The formalism allows to extract the fractional spherical occupancies of the orbitals in the valence space. The structure of the three 0_1^+ , 3_1^+ and 8_1^- states is shown in Table III. with a possible large mixing of spherical orbital our description is richer than single quasi-particle estimates which are often used to assign excited and isomeric states to a single excited configurations. This is reflected in the partial occupancies of the whole proton and neutron orbitals involved in the valence space. Nevertheless, one can point out that both for protons and neutrons, the fillings proceed through the "largest" orbitals and that excited 3_1^+ and 8_1^- states mainly differ from the ground state by an additional proton particle filling the $1h_{9/2}$ orbital, assigning these states as having a "proton" nature. We may recall here that we obtain an excellent reproduction of the experimental data with no adjustment of the effective interaction, designed more than two decades ago. Nevertheless, in order to confirm

the present outcome from our calculations, a broader systematic study has been developed, and in particular we would like to connect the slight energy shift of the $K^\pi = 3^+$ multiplet to a specific single particle monopole drift for a better reproductive and predictive description of the overall region.

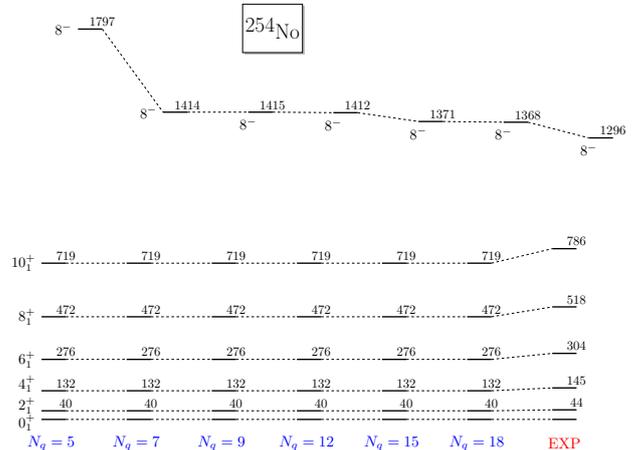


FIGURE 7: Evolution of the lower part of ^{254}No spectrum with respect to the number of HF states found by the minimization procedure.

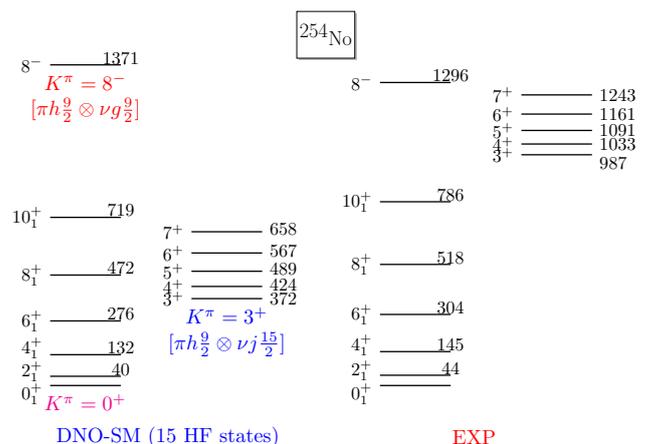


FIGURE 8: Comparison of DNO-SM calculation using 15 HF states with the experimental spectrum.

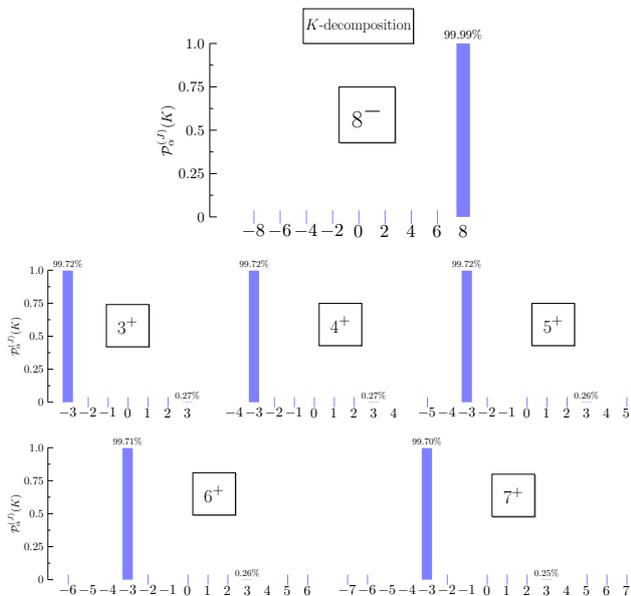


FIGURE 9: K -quantum number content of the isomeric 3^+ band and the 8^- state.

proton orbits	$1h_{9/2}$	$1i_{13/2}$	$2f_{7/2}$	$2f_{5/2}$	$3p_{3/2}$	$3p_{1/2}$	
0_1^+	5.66	7.99	3.44	1.58	0.76	0.57	
8^-	6.52	7.82	3.28	1.20	0.79	0.39	
3^+	6.50	7.98	3.31	1.14	0.72	0.35	
neutron orbits	$1i_{11/2}$	$1j_{15/2}$	$2g_{9/2}$	$2g_{7/2}$	$3d_{5/2}$	$3d_{3/2}$	$4s_{1/2}$
0_1^+	7.28	9.67	5.45	1.11	1.16	0.87	0.46
8^-	7.29	9.04	6.07	1.12	1.15	0.88	0.45
3^+	7.31	9.94	5.43	0.99	1.07	0.83	0.43

TABLE III: Occupancies of the spherical orbitals for the ground state and 8^- and 3^+ states.

V. CONCLUSION AND PERSPECTIVES

As a summary, in this paper we have exposed the formalism of the DNO-SM which amounts to diagonalize

shell-model hamiltonians in a non-orthogonal basis with the use of beyond-mean-field techniques. Particular effort has been put into the proper selection of optimal basis state used for the diagonalisation. We benchmarked the method over a large set of sd shell nuclei and could reproduce the energies, and transitions probabilities of the exact diagonalisations at the cost of very few basis states. For the first time, we applied the DNO-SM method to a superheavy system ^{254}No which is obviously far beyond the capabilities of actual diagonalisations codes. The DNO-SM formalism has also recently been very useful in the interpretation of several experimental studies [34–37] and has been to be extremely promising both for intrinsic interpretation of shell-model diagonalisations, and setting new frontiers for nuclear structure studies within the shell-model framework.

VI. ACKNOWLEDGMENTS

The authors would like to dedicate the present work to the memory of the late Etienne Caurier, who was at the initiative of the present developments.

Annexe A: Matrix elements in the PCHF basis

Considering the two-body Hamiltonian $\hat{\mathcal{H}}$ defined in (2), in the PCHF basis $\mathcal{P}_{MK}^J |\Phi(q)\rangle \in \Gamma_0$, it is represented by the set of matrix elements $\langle \Phi(q') | \hat{\mathcal{H}} \mathcal{P}_{K'K}^J |\Phi(q)\rangle$ given by (15). The calculation of this matrix element requires an evaluation of the hamiltonian kernel which, for two arbitrary Slater determinants $|\Phi'\rangle$ and $|\Phi\rangle$, takes the forms (cf. e.g. Ref. [25])

$$\langle \Phi' | \hat{\mathcal{H}} \hat{R}(\Omega) | \Phi \rangle = \sum_{\substack{p \in \Phi' \\ q \in \Phi}} (-)^{p+q} M_{pq}(\Omega) \langle p | \hat{E} \hat{R}(\Omega) | q \rangle + \sum_{\substack{p < q \in \Phi' \\ r < s \in \Phi}} (-)^{p+q+r+s} M_{pqrs}(\Omega) \langle pq | \hat{\mathcal{V}} \hat{R}(\Omega) | rs \rangle \quad (\text{A1})$$

where $M_{pq}(\Omega)$, $M_{pqrs}(\Omega)$ are respectively first- and second-order minors of the $A \times A$ matrix $N(\Omega) = D^\dagger \cdot R(\Omega) \cdot D$ with a rectangular matrix $D_{ip} = \{C_i^{(p)}, p \in \Phi, i \in \mathcal{E}\}$ representing the single particle HF states in the

Slater $|\Phi\rangle$. The matrix element of the one-body single-particle energy \hat{E} is given by

$$\langle p | \hat{E} \hat{R}(\Omega) | q \rangle = \sum_{i_1, i_2, i \in \mathcal{E}} C_{i_1}^{(p)} C_{i_2}^{(q)} e_{i_1 i} R_{i i_2}(\Omega). \quad (\text{A2})$$

Whereas for the two-body term, it is written in terms of the antisymmetrized matrix element

$\langle JT(i_1 i_2) | \hat{\mathcal{V}} | JT(i_3 i_4) \rangle$ of good angular momentum and isospin J, T

$$\langle pq | \hat{\mathcal{V}} \hat{R}(\Omega) | rs \rangle = \sum_{\substack{JMM' \\ TT_z \\ i_1 i_2 i_3 i_4}} C_{\frac{1}{2}\tau_p \frac{1}{2}\tau_q}^{TT_z} C_{\frac{1}{2}\tau_r \frac{1}{2}\tau_s}^{TT_z} C_{j_1 m_1 j_2 m_2}^{JM} C_{j_3 m_3 j_4 m_4}^{JM'} \mathcal{D}_{MM'}^J(\Omega) C_{i_1}^{(p)} C_{i_2}^{(q)} C_{i_3}^{(r)} C_{i_4}^{(s)} \langle JT(i_1 i_2) | \hat{\mathcal{V}} | JT(i_3 i_4) \rangle. \quad (\text{A3})$$

Here $C_{j_1 m_1 j_2 m_2}^{JM}$ is the Clebsch–Gordan coefficient.

Annexe B: Derivation of the analytical integration over the Euler angles α, γ

Appendix A provides the necessary elements we need to derive an analytical formula for the integrations over α, γ in (15). For that goal, we just need to perform the derivation with $\hat{O} = \mathbb{K}$, the same procedure holds for other operators such as the Hamiltonian or transition operators. In this case, we have the norm matrix element

$$\mathcal{N}_{K'K}^J = \frac{2J+1}{4\pi^2(3-(-)^A)} \int d\Omega \mathcal{D}_{MK}^{J*}(\Omega) \det N(\Omega) \quad (\text{B1})$$

where we have used the equality $\det N(\Omega) = \langle \Phi' | \hat{R}(\Omega) | \Phi \rangle$. Let us rewrite this quantity in an explicit way with a summation over all permutations σ of the permutation group of A -particles S_A

$$\begin{aligned} \det N &= \sum_{\sigma \in S_A} \text{sgn}(\sigma) \prod_{\lambda=1}^A N_{\lambda, \sigma(\lambda)} \\ &= \sum_{\sigma \in S_A} \text{sgn}(\sigma) \prod_{\lambda=1}^A \left(\sum_{i_1 i_2 \in \mathcal{E}} D'_{\lambda i_1} R_{i_1 i_2} D_{i_2 \sigma(\lambda)} \right) \\ &= \sum_{\substack{i_1(1) i_2(1) \\ \dots \\ i_1(A) i_2(A)}} \prod_{\lambda=1}^A D'_{\lambda i_1(\lambda)} \prod_{\lambda=1}^A R_{i_1(\lambda) i_2(\lambda)} \\ &\quad \left(\sum_{\sigma \in S_A} \text{sgn}(\sigma) \prod_{\lambda=1}^A D_{i_2(\lambda) \sigma(\lambda)} \right). \end{aligned} \quad (\text{B2})$$

The norm matrix element thus becomes

$$\begin{aligned} \mathcal{N}_{K'K}^{(J)} &= \frac{2J+1}{4\pi^2(3-(-)^A)} \sum_{\substack{i_1(1) i_2(1) \\ \dots \\ i_1(A) i_2(A)}} \\ &\quad \prod_{\lambda=1}^A D'_{\lambda i_1(\lambda)} \left(\sum_{\sigma \in S_A} \text{sgn}(\sigma) \prod_{\lambda=1}^A D_{i_2(\lambda) \sigma(\lambda)} \right) \times \\ &\quad \int d\Omega \mathcal{D}_{MK}^{J*}(\Omega) \prod_{\lambda=1}^A R_{i_1(\lambda) i_2(\lambda)}(\Omega). \end{aligned} \quad (\text{B3})$$

In this form, the integration over Euler angles $\Omega = (\alpha, \beta, \gamma)$ is isolated and can be subject to a direct evaluation using the rotation matrix in spherical oscillator basis $R_{i_1 i_2}(\Omega) = e^{-i\alpha m_1} d_{m_1 m_2}^j(\beta) e^{-i\gamma m_2}$. Hence, one can write

$$\begin{aligned} &\int d\Omega \mathcal{D}_{MK}^{J*}(\Omega) \prod_{\lambda=1}^A R_{i_1(\lambda) i_2(\lambda)}(\Omega) \\ &= \int_0^{2\pi} d\alpha e^{i\alpha [K' - \sum_{\lambda=1}^A m_1(\lambda)]} \int_0^{\gamma_{\max}} d\gamma e^{i\gamma [K - \sum_{\lambda=1}^A m_2(\lambda)]} \\ &\quad \int_0^{\pi} d\beta \sin \beta d_{K'K}^{*J}(\beta) \prod_{\lambda=1}^A d_{m_1(\lambda) m_2(\lambda)}^{j(\lambda)}(\beta) \end{aligned} \quad (\text{B4})$$

from which it is trivial to calculate the integrals over α, γ . The result simply reads

$$\begin{aligned} &\int d\Omega \mathcal{D}_{MK}^{J*}(\Omega) \prod_{\lambda=1}^A R_{i_1(\lambda) i_2(\lambda)}(\Omega) = 2\pi \gamma_{\max} \times \\ &\quad \delta_{\Delta K', 0} \delta_{\Delta K, 0} \int_0^{\pi} d\beta \sin \beta d_{K'K}^{*J}(\beta) \prod_{\lambda=1}^A d_{m_1(\lambda) m_2(\lambda)}^{j(\lambda)}(\beta) \end{aligned} \quad (\text{B5})$$

where we denote $\Delta K' = K' - \sum_{\lambda=1}^A m_1(\lambda)$ and $\Delta K = K - \sum_{\lambda=1}^A m_2(\lambda)$. This form is of course not practical as it involves summations over $A!$ permutations. Our next step is to recast it into the familiar expression as in (B1) with only the integration over β being left to evaluate. To do so, notice that

$$\delta_{n,0} = \frac{1}{N} \sum_{k=1}^N e^{i \frac{2\pi k}{N} n} \text{ if } \begin{cases} N \in \mathbb{N}, N \geq 2, \\ n \in \mathbb{Z}, e^{i \frac{2\pi}{N} n} \neq 1. \end{cases} \quad (\text{B6})$$

It is obvious that $\Delta K', \Delta K \in \mathbb{Z}$ regardless the odd or even mass number A so that applying this identity allows

us to obtain

$$\int d\Omega \mathcal{D}_{MK}^{J*}(\Omega) \prod_{\lambda=1}^A R_{i_1(\lambda)i_2(\lambda)}(\Omega) = \frac{2\pi\gamma_{\max}}{N_\alpha N_\gamma} \times \sum_{k_1=1}^{N_\alpha} \sum_{k_2=1}^{N_\gamma} \int_0^\pi d\beta \sin \beta \mathcal{D}_{K'K}^{*J}\left(\frac{2\pi k_1}{N_\alpha}, \beta, \frac{2\pi k_2}{N_\gamma}\right) \times \prod_{\lambda=1}^A R_{i_1(\lambda)i_2(\lambda)}\left(\frac{2\pi k_1}{N_\alpha}, \beta, \frac{2\pi k_2}{N_\gamma}\right) \quad (\text{B7})$$

where $N_\alpha, N_\gamma \in \mathbb{Z}$ are chosen according to the condition (B6). The final expression of the norm matrix ele-

ment thus reads

$$\mathcal{N}_{K'K}^J = \frac{2J+1}{2} \cdot \frac{1}{N_\alpha N_\gamma} \sum_{k_1=1}^{N_\alpha} \sum_{k_2=1}^{N_\gamma} \int_0^\pi d\beta \sin \beta \times \mathcal{D}_{K'K}^{*J}\left(\frac{2\pi k_1}{N_\alpha}, \beta, \frac{2\pi k_2}{N_\gamma}\right) \times \det N\left(\frac{2\pi k_1}{N_\alpha}, \beta, \frac{2\pi k_2}{N_\gamma}\right). \quad (\text{B8})$$

The same reasoning leaves us with the Hamiltonian matrix element where α, γ are exactly integrated out

$$\mathcal{H}_{K'K}^J = \frac{2J+1}{2} \cdot \frac{1}{N_\alpha N_\gamma} \sum_{k_1=1}^{N_\alpha} \sum_{k_2=1}^{N_\gamma} \int_0^\pi d\beta \sin \beta \mathcal{D}_{K'K}^{*J}\left(\frac{2\pi k_1}{N_\alpha}, \beta, \frac{2\pi k_2}{N_\gamma}\right) \langle \Phi' | \hat{\mathcal{H}} \hat{R}\left(\frac{2\pi k_1}{N_\alpha}, \beta, \frac{2\pi k_2}{N_\gamma}\right) | \Phi \rangle. \quad (\text{B9})$$

$N_u(u = \alpha, \gamma)$ will be chosen to ensure the conditions

$$e^{i\frac{2\pi}{N_u}\Delta K_v} \neq 1 \quad \forall v = 0, 1, 2 \text{ with } \begin{cases} \Delta K_0 = K - \sum_{\lambda=1}^A m_i(\lambda) & \forall i \in \mathcal{E} \\ \Delta K_1 = K - m_i - \sum_{\lambda=1}^{A-1} m_{i'}(\lambda) & \forall i, i' \in \mathcal{E} \\ \Delta K_2 = K - M(i_1, i_2) - \sum_{\lambda=1}^{A-2} m_i(\lambda) & \forall i, i_1, i_2 \in \mathcal{E} \end{cases} \quad (\text{B10})$$

with i_1, i_2 designating two single-particle harmonics oscillator states coupled to a total angular momentum

$$M = m_{i_1} + m_{i_2}.$$

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