HARTREE–FOCK CALCULATIONS IN THE CONFINED PLANE-WAVE BASIS WITH A GENERAL NUCLEON–NUCLEON INTERACTION*

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We present a single-particle basis made of plane-wave states confined in a cubic box designed for Hartree–Fock calculations using a general nuclear two-body interaction with triaxial self-consistent symmetry. We show that this basis allows to calculate two-body nuclear potential matrix elements without recourse to center-of-mass transformations and to calculate exactly Coulomb interaction matrix elements in an economical way. Using various two-body nuclear interactions, we study the Hartree–Fock convergence with the two basis parameters: the cubic edge length and a spherical momentum truncation. We show that the former can be determined by the nuclear radius and the latter is essentially related to the momentum cutoff of the nuclear interaction.

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1. Introduction

The Hartree–Fock approximation is very successful in describing ground state bulk properties of nuclei over the nuclear chart [1], especially when one needs to take into account deformation properties. With recent progress of non-empirical nuclear interactions [2], it becomes desirable to treat a general internucleon potential at the Hartree–Fock level which is usually a starting point in more sophisticated many-body methods. As it is well known in this approach, a crucial point is the choice of the representation basis. In this work, we will present a single-particle basis made of plane-wave states confined in a cubic box and show that (i) the treatment of a general two-body nuclear interaction is straightforward if one knows its momentum

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representation (which is usually the case for non-empirical interactions), (*ii*) this basis allows an exact treatment of the Coulomb interaction, and (*iii*) it can conveniently be used to construct symmetry-adapted bases which are necessary in implementing symmetries in mean-field approaches (self-consistent or not).

2. Confined plane-wave basis

2.1. Construction of the basis

Let us consider the one-dimensional plane-wave equation

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,\varphi(x) + k^2\,\varphi(x) = 0 \tag{1}$$

with $k \in \mathbb{R}$. The normalized plane wave $\varphi(x)$ is required to satisfy the confinement condition

$$\varphi(x) = \begin{cases} \dfrac{1}{\sqrt{L}}\,\mathrm{e}^{ikx}\,, & x \in \left[-\dfrac{L}{2}, \dfrac{L}{2}\right] \\ 0 \quad , & |x| > \dfrac{L}{2}\,, \end{cases} \tag{2}$$

where $L > 0$ defines the cubic edge length. Moreover, let us impose that the plane-waves $\{\varphi(x)\}$ are orthonormal in $[-L/2, L/2]$, hence,

$$\frac{1}{L}\int\limits_{-L/2}^{L/2} \mathrm{d}x\,\mathrm{e}^{i(k_1-k_2)x} = \delta_{k_1 k_2}\,, \qquad k_1, k_2 \in \mathbb{R}\,. \tag{3}$$

This condition implies $k_1 - k_2 = m\,\frac{2\pi}{L}$, with $m \in \mathbb{Z}$, and we note that this condition is satisfied in particular by two disjoint sets of orthornormal confined plane-waves of the form of

$$\varphi_m(x) = \frac{1}{\sqrt{L}}\,\mathrm{e}^{ik_m x}\,, \qquad x \in \left[-\frac{L}{2}, \frac{L}{2}\right] \tag{4}$$

with $k_m = m\dfrac{2\pi}{L}$. The first set is characterized by $m \in \mathbb{Z}$ and the second by $m - \frac{1}{2} \in \mathbb{Z}$. Using the Dirac notation, we define the confined plane-wave state $|\varphi_m\rangle$ by $\langle x\,|\,\varphi_m\rangle = \varphi_m(x)$. Accordingly, in the three-dimensional case, one can define the confined plane-wave state of momentum $\boldsymbol{k}_\alpha = \frac{2\pi}{L}(\alpha_x, \alpha_y, \alpha_z)$ as

$$\langle \boldsymbol{r}\,|\,\varphi_\alpha\rangle = \begin{cases} \dfrac{1}{L^{3/2}}\,\mathrm{e}^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}}, & \boldsymbol{r} \in \left[-\dfrac{L}{2}, \dfrac{L}{2}\right]^3\,, \\ 0 \quad , & \text{otherwise}\,. \end{cases} \tag{5}$$

The index α thus refers to the triplet of indices $(\alpha_x, \alpha_y, \alpha_z)$. In the following, we will consider the states including spin $\{|\varphi_\alpha \sigma\rangle\}$ ($\sigma = \pm\frac{1}{2}$) and call it the confined plane-wave basis. Apart from a different approach to derive it, this basis is similar to that considered by van Dalen and Müther in Ref. [3].

2.2. Symmetry-adapted basis

The confinement of plane waves in a cubic box implies that the resulting states $\{|\varphi_\alpha \sigma\rangle\}$ transform among themselves under the full octahedral double group with time-reversal symmetry, denoted by $O_{2\mathrm{h}}^{\mathrm{DT}}$ (as in Ref. [4]). It is a subgroup of the direct product $\mathrm{SU}(2) \times \mathrm{Gr}\{\hat{T}\}$, where $\hat{T}$ is the time-reversal operator, so spherical and axial symmetries are broken. Moreover, we choose its subgroup $G_{\mathrm{sc}} = \mathrm{Gr}\{\hat{\Pi}, \hat{R}_z, \hat{R}_y^T\}$ as the group of self-consistent symmetries of the Hartree–Fock Hamiltonian, where $\hat{\Pi}$ is the intrinsic parity operator, $\hat{R}_m$ is the m-signature operator, namely the rotation operator of angle π about the axis m (x, y or z), and $\hat{R}_y^T = \hat{T}\hat{R}_y$. This choice allows to describe time-reversal symmetry breaking by the mean field, as in odd-mass nuclei, but because the confined plane-wave basis is invariant under $O_{2\mathrm{h}}^{\mathrm{DT}}$, it is also possible to describe time-reversal invariant solutions as in the ground state of even–even nuclei. Even if we consider the latter cases only, it is more advantageous not to add $\hat{T}$ to the above self-consistent symmetry group G_{sc}, which would yield the full dihedral double group with time-reversal symmetry $D_{2\mathrm{h}}^{\mathrm{DT}}$. Indeed the unitary subgroup $\mathrm{Gr}\{\hat{\Pi}, \hat{R}_z\}$ of G_{sc} is Abelian and yields two quantum numbers (intrinsic parity and z-signature), whereas the unitary subgroup $\mathrm{Gr}\{\hat{\Pi}, \hat{R}_z, \hat{R}_y\}$ of $D_{2\mathrm{h}}^{\mathrm{DT}}$ is non-Abelian and yields only one quantum number (intrinsic parity). Moreover, in both cases, one can reduce the set of discretized momenta to one eighth of the full three-dimensional mesh in order to generate a basis of reducible corepresentation of $O_{2\mathrm{h}}^{\mathrm{DT}}$.

The symmetry-adapted basis in the present case is obtained by a proper unitary transformation of the above-defined confined plane-wave basis. It can be constructed through the use of projection operators $\hat{P}(p) = \frac{1}{2}\left(\mathbb{1} + \frac{\hat{\Pi}}{p}\right)$ and $\hat{P}(r_z) = \frac{1}{2}\left(\mathbb{1} + \frac{\hat{R}_z}{r_z}\right)$, where $p = \pm 1$ and $r_z = \pm i$ are the intrinsic-parity and z-signature quantum numbers. Moreover, defining the operator $\hat{Q}_c = \frac{1}{2}(\mathbb{1} + c\hat{R}_y^T)$, with $c = \pm 1$, one can show that for fixed (p, r_z), $\alpha = (\alpha_x, \alpha_y, \alpha_z)$, with $\alpha_m - \frac{1}{2} \in \mathbb{N}$ ($m = x, y, z$) and $\sigma = \pm\frac{1}{2}$, the two states

$$|p, r_z(c\alpha\sigma)\rangle = \sqrt{8}\, \hat{P}(p)\hat{P}(r_z)\hat{Q}_c\, |\varphi_\alpha, \sigma\rangle\,, \qquad c = \pm 1\,, \tag{6}$$

form two bases of equivalent irreducible corepresentations of G_{sc} of dimension 1. Note that here we have chosen to work with α being a half-integer triplet, therefore, all α_m indices are different from 0.

2.3. Truncation of the basis

The confined plane-wave basis $\{|\varphi_\alpha \sigma\rangle\}$ is characterized by the discrete equidistant momenta $\boldsymbol{k}_\alpha = \frac{2\pi}{L}(\alpha_x, \alpha_y, \alpha_z)$ where we have chosen the set of half-integer triplets indexed by α. Since, in practice, it is necessary to work with a finite set of states, we introduce a parameter Λ_b so as to select basis states of momenta $\|\boldsymbol{k}_\alpha\| \leqslant \Lambda_\mathrm{b}$. The confined plane-wave basis can thus be described by two parameters: the box size L and the spherical momentum truncation Λ_b. Since this truncation is applied to the norm of the momentum vectors, it preserves the octahedral symmetry of the confined plane-wave basis and the construction of the symmetry-adapted basis is unaffected.

3. Hartree–Fock approximation in the symmetry-adapted confined plane-wave basis

3.1. Nuclear Hamiltonian and Hartree–Fock Hamiltonian

Let us denote by $\hat{K}$ the total kinetic-energy (one-body) operator and make the approximation that all nucleons have the same mass m. The intrinsic kinetic-energy operator $\hat{K}_\mathrm{intr} = \hat{K} - \frac{\hat{\boldsymbol{P}}^2}{2Am}$ (representing the kinetic energy of the nucleus of mass number A in its center-of-mass frame) can be written as $\hat{K}_\mathrm{intr} = \hat{K} - \hat{K}_1 - \hat{K}_2$, where $\hat{K}_1$ and $\hat{K}_2$ are the one-body and two-body corrections to the total kinetic energy and are defined by

$$\hat{K}_1 = \frac{1}{A}\,\hat{K}\,, \qquad \hat{K}_2 = \frac{1}{2Am}\sum_{i\neq j}\hat{\boldsymbol{p}}_i \cdot \hat{\boldsymbol{p}}_j\,, \tag{7}$$

where $\hat{\boldsymbol{p}}_i$ is the momentum operator of the nucleon i. The Hamiltonian of the nucleus is thus $\hat{H} = \hat{K}_\mathrm{intr} + \hat{V}$, where $\hat{V}$ denotes the sum of the two-body nuclear and Coulomb interactions. The one-body Hartree–Fock Hamiltonian can be then written in the form of

$$\hat{h}_\mathrm{HF} = \left(1 - \frac{1}{A}\right)\frac{\hat{\boldsymbol{p}}^2}{2m} + \hat{v}_\mathrm{HF}\,, \tag{8}$$

where the Hartree–Fock potential $\hat{v}_\mathrm{HF}$ is defined as the one-body reduction of the two-body operator $\hat{V} - \hat{K}_2$ for the Slater determinant $|\Phi\rangle$ solution to the Hartree–Fock equations. This treatment of the center-of-mass correction thus corresponds to the full correction (A) discussed in Ref. [5].

Assuming that isospin projection τ is a good quantum number, Eq. (8) can be solved separately for neutrons and protons. The matrix elements of the Hartree–Fock potential $\hat{v}_{\rm HF}$ for a fixed value of τ are calculated in the symmetry-adapted confined plane-wave basis (6) as

$$\begin{aligned}
&\langle\, p, r_z\left(c'\alpha'\sigma'\right)|\hat{v}^{(\tau)}_{\rm HF}|p, r_z(c\alpha\sigma)\,\rangle \\
&= \sum_{\tau',p',r'_z}\sum_{\substack{c'_2\alpha'_2\sigma'_2\\ c_2\alpha_2\sigma_2}} \langle\, p', r'_z(c_2\alpha_2\sigma_2)\tau'|\hat{\rho}|p', r'_z\left(c'_2\alpha'_2\sigma'_2\right)\tau'\,\rangle \\
&\times \langle\, p, r_z\left(c'\alpha'\gamma'\right)\tau; p', r'_z(c'_2\alpha'_2\sigma'_2)\tau'|\left(\hat{V}-\hat{K}_2\right) \\
&\times \left(\mathbb{1}-\hat{P}_{12}\right)|p, r_z(c\alpha\sigma)\tau; p', r'_z(c_2\alpha_2\sigma_2)\tau'\,\rangle\,, \qquad (9)
\end{aligned}$$

where $\hat{P}_{12}$ denotes here the permutation operator of two-body states. The operator $\hat{\rho}$ is the one-body density associated to the Slater determinant $|\Phi\rangle$.

3.2. Nuclear and Coulomb interaction matrix elements

The matrix element of a Galilean- and translationally invariant two-body interaction $\hat{V}$ between confined plane-wave states is calculated through the coordinate representation of these states as

$$\begin{aligned}
\langle\, \varphi_{\alpha'_1}\varphi_{\alpha'_2}|\hat{V}|\varphi_{\alpha_1}\varphi_{\alpha_2}\,\rangle &= \int\limits_{\mathbb{R}^3}\mathrm{d}\boldsymbol{R}\int\limits_{\mathbb{R}^3}\mathrm{d}\boldsymbol{r}'\int\limits_{\mathbb{R}^3}\mathrm{d}\boldsymbol{r}\Big\langle\varphi_{\alpha'_1}\Big|\boldsymbol{R}+\frac{\boldsymbol{r}'}{2}\Big\rangle \\
\times\Big\langle\varphi_{\alpha'_2}\Big|\boldsymbol{R}-\frac{\boldsymbol{r}'}{2}\Big\rangle\Big\langle\boldsymbol{r}'|\hat{V}|\boldsymbol{r}\Big\rangle\,\Big\langle\boldsymbol{R}+\frac{\boldsymbol{r}}{2}\Big|\varphi_{\alpha_1}\Big\rangle\Big\langle\boldsymbol{R}-\frac{\boldsymbol{r}}{2}\Big|\varphi_{\alpha_2}\Big\rangle\,. \qquad (10)
\end{aligned}$$

Let us denote the cubic domain $\mathcal{D}=[-L,L]^3$. Then, confinement condition (2) leads to the following restriction on integration variables: $\boldsymbol{r}',\boldsymbol{r}\in\mathcal{D}$ and $\boldsymbol{R}\in\mathcal{D}_{\boldsymbol{r}'}\cap\mathcal{D}_{\boldsymbol{r}}$ where $\mathcal{D}_{\boldsymbol{r}}=\mathcal{D}_x\times\mathcal{D}_y\times\mathcal{D}_z$ with, for instance, $\mathcal{D}_x=\Big[-\frac{L}{2}+\frac{|x|}{2},\frac{L}{2}-\frac{|x|}{2}\Big]$.

Suppose that the box size L is large enough comparing to the range of the nuclear interaction $\hat{V}_{NN}$. The variation domain of the center-of-mass coordinate $\boldsymbol{R}$ can be considered to be independent of the relative distances, *i.e.*, $\mathcal{D}_x\approx[-L/2,L/2]$. This allows us to write (10) in the coordinate representation of three-dimensional confined plane-wave basis as

$$\begin{aligned}
\langle\, \varphi_{\alpha'_1}\varphi_{\alpha'_2}|\hat{V}_{NN}|\varphi_{\alpha_1}\varphi_{\alpha_2}\,\rangle &\approx \left(\frac{1}{L^3}\int\limits_{[-L/2,L/2]^3}\mathrm{e}^{i(\boldsymbol{K}_{\alpha'}-\boldsymbol{K}_{\alpha})\cdot\boldsymbol{R}}\right) \\
\times\frac{1}{L^3}\int\limits_{\mathcal{D}}\mathrm{d}^3\boldsymbol{r}'\,\mathrm{e}^{-i\boldsymbol{k}_{\alpha'}\cdot\boldsymbol{r}r'}\int\limits_{\mathcal{D}}\mathrm{d}^3\boldsymbol{r}\,\mathrm{e}^{i\boldsymbol{k}_{\alpha}\cdot\boldsymbol{r}}\,\langle\,\boldsymbol{r}'|\hat{V}_{NN}|\boldsymbol{r}\,\rangle\,, \qquad (11)
\end{aligned}$$

with the relative and center-of-mass momenta

$$\begin{cases} \boldsymbol{k}_\alpha = \frac{1}{2}\left(\boldsymbol{k}_{\alpha_1} - \boldsymbol{k}_{\alpha_2}\right) , \\ \boldsymbol{K}_\alpha = \boldsymbol{k}_{\alpha_1} + \boldsymbol{k}_{\alpha_2} , \end{cases} \qquad \begin{cases} \boldsymbol{k}_{\alpha'} = \frac{1}{2}\left(\boldsymbol{k}_{\alpha'_1} - \boldsymbol{k}_{\alpha'_2}\right) , \\ \boldsymbol{K}_{\alpha'} = \boldsymbol{k}_{\alpha'_1} + \boldsymbol{k}_{\alpha'_2} . \end{cases} \tag{12}$$

Note that in Eq. (11), the integral over the center-of-mass coordinate $\boldsymbol{R}$ is the overlap of confined plane-wave states of momenta $\boldsymbol{K}_{\alpha'}$ and $\boldsymbol{K}_\alpha$. Moreover, because of the large box size in comparison with the interaction range, the remaining integrals in the coordinate space can be approximated by the momentum representation of $\hat{V}_{NN}$. Thus, we end up with the approximation

$$\langle\, \varphi_{\alpha'_1}\varphi_{\alpha'_2}|\hat{V}_{NN}|\varphi_{\alpha_1}\varphi_{\alpha_2}\,\rangle \approx \delta_{\alpha'_1+\alpha'_2,\alpha_1+\alpha_2} \left(\frac{2\pi}{L}\right)^3 \langle\, \boldsymbol{k}_{\alpha'}|\hat{V}_{NN}|\boldsymbol{k}_\alpha\,\rangle . \tag{13}$$

Therefore, in the confined plane-wave basis, the two-body nuclear matrix elements are simply proportional to the momentum representation of the interaction. This is in constrast with other bases, such as the partial-wave or harmonic-oscillator basis, where it is neccessary to perform a transformation from the laboratory frame to the center-of-mass frame using vector brackets [6] or Moshinsky coefficients [7].

Let us now consider the case of the Coulomb interaction. Since this interaction has an infinite range, the approximation above does not hold. The center-of-mass motion will be directly integrated out. Due to the locality of the Coulomb interaction, (10) is simplified into

$$\langle\, \varphi_{\alpha'_1}\varphi_{\alpha'_2}|\hat{V}_{\text{Coul}}|\varphi_{\alpha_1}\varphi_{\alpha_2}\,\rangle = \frac{e^2}{L^6}\int\limits_{\mathcal{D}} \mathrm{d}^3\boldsymbol{r} \left(\frac{\mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{r}}}{\|\boldsymbol{r}\|}\int\limits_{\mathcal{D}_{\boldsymbol{r}}} \mathrm{d}^3\boldsymbol{R}\,\mathrm{e}^{i\boldsymbol{Q}\cdot\boldsymbol{R}}\right) , \tag{14}$$

where we have introduced the transfer momenta

$$\begin{cases} \boldsymbol{q} = \frac{1}{2}\left(\boldsymbol{k}_{\alpha'_1} - \boldsymbol{k}_{\alpha'_2}\right) - \frac{1}{2}\left(\boldsymbol{k}_{\alpha'_1} - \boldsymbol{k}_{\alpha'_2}\right) , \\ \boldsymbol{Q} = \left(\boldsymbol{k}_{\alpha'_1} + \boldsymbol{k}_{\alpha'_2}\right) - \left(\boldsymbol{k}_{\alpha_1} + \boldsymbol{k}_{\alpha_2}\right) . \end{cases} \tag{15}$$

To calculate the Coulomb matrix element in the confined plane-wave basis, one can, therefore, integrate out the center-of-mass motion analytically, whereas the singularity at the origin can be treated using the spherical coordinates

$$\langle\, \varphi_{\alpha_1'}\varphi_{\alpha_2'}|\hat{V}_{\rm Coul}|\varphi_{\alpha_1}\varphi_{\alpha_2}\,\rangle = 8\,\frac{e^2}{L^6}\times$$
$$\int_{\mathcal{D}_{\rm c}}\!\!{\rm d}\varphi\,{\rm d}\theta\,\sin\theta\,{\rm d}r\,r\,\cos(x\,q_x)\cos(y\,q_y)\cos(z\,q_z)\,f(Q_x,|x|)\,f(Q_y,|y|)\,f(Q_z,|z|), \tag{16}$$

where $\mathcal{D}_{\rm c}$ is a cube defined in Cartesian coordinates by $[0;L]^3$, Q_x, Q_y, Q_z are the Cartesian components of $\boldsymbol{Q}$, and the function f is defined by $f(Q,x) = (L-x)\,\mathrm{sinc}\Big(\frac{Q(L-x)}{2}\Big)$.

Before closing this section, it is important to note that, from definition (12) of relative momenta and because of the cutoff $\Lambda_{\rm b}$ imposed on single-particle momenta, the relative-momentum mesh points at which we evaluate the nuclear interaction matrix elements in Eq. (13) is also bounded by $\Lambda_{\rm b}$. Moreover, the equidistance of single-particle momentum values for a fixed box size L results in a number of matrix elements $\langle\, \boldsymbol{k}_{\alpha'}|\hat{V}_{NN}|\boldsymbol{k}_{\alpha}\,\rangle$ to be computed and stored which is only of the order of N^2, where N is the number of single-particle momentum mesh points. As for the Coulomb interaction matrix elements in the confined plane-wave basis, the norms of transfer momenta $\boldsymbol{q}_\alpha$ and $\boldsymbol{Q}_\alpha$ at play are bounded by $2\Lambda_{\rm b}$ and $4\Lambda_{\rm b}$, respectively, and a scaling reduction resulting from the equidistance of the momentum mesh also occurs. This feature is essential to make the present triaxial-deformed Hartree–Fock calculations tractable and more economical than in the partial-wave or harmonic-oscillator basis.

4. Numerical results of Hartree–Fock calculations

4.1. Convergence of Hartree–Fock solutions with basis parameters

We are now in a position to address the convergence of Hartree–Fock solutions in the confined plane-wave basis. To find a criterion on the choice of the basis parameters $(L,\Lambda_{\rm b})$, it is worth noting that (*i*) the box size should be larger than the nuclear size, *i.e.*, one can use for instance the nuclear charge radius $r_{\rm c}$ and take $L = \alpha \times r_{\rm c}$, where the factor α is to be estimated, and (*ii*) if the nuclear interaction has some momentum cutoff Λ_{NN}, then one should have $\Lambda_{\rm b} \gtrsim \Lambda_{NN}$. In this subsection, we disregard the two-body center-of-mass correction as it is not expected to alter the conclusions about the dependence on basis parameters of the Hartree–Fock solution.

We first consider the density-independent SV parametrization of Skyrme force [8] and omit the Coulomb interaction. Table I shows the binding energy of ^{16}O calculated as a function of the confined plane-wave basis parameters L and $\Lambda_{\rm b}$.

TABLE I

Binding energy (in MeV) of ^{16}O with the SV parametrization for different pairs of (L, Λ_b) parameter values.

L	Λ_b 2.0	2.5	3.0
15.0	−126.685	−126.915	−127.230
17.5	−126.675	−126.895	−127.208
20.0	−126.669	−126.910	−127.010

Although the convergence in L for a fixed cutoff Λ_b is not monotonic, smaller boxes are found to generally yield overbinding. In contrast Λ_b being a variational parameter, the binding energy is found to be a decreasing function of Λ_b as exptected. Figure 1 presents the binding energy as a function of L over an extended interval with $\Lambda_b = 2.0$ fm^{-1}. As the experimental charge radius of ^{16}O is about 2.7 fm, the parameter L can be chosen at least about 4 to 5 times r_c in this case.

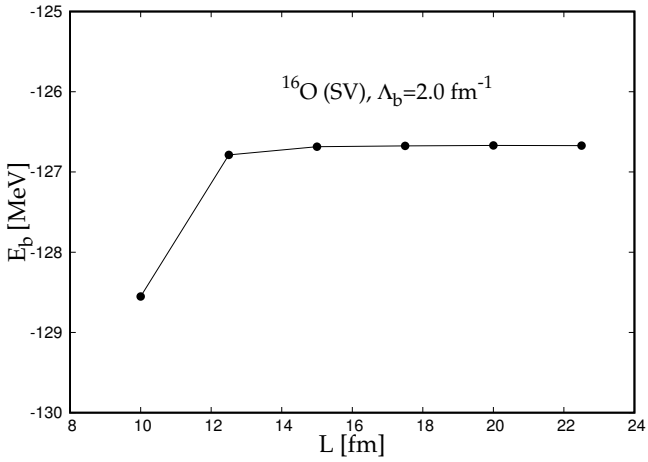

Fig. 1. Hartree–Fock binding energy of ^{16}O as a function of the cubic edge length L with the Skyrme SV interaction, without Coulomb interaction and two-body kinetic-energy correction, and using $\Lambda_b = 2.0$ fm^{-1}.

Next, we explore the convergence with basis parameters of Hartree–Fock solutions obtained with a non-empirical interaction. We report in Table II the binding energy and charge radius of ^{16}O calculated as a function of the basis truncation parameter Λ_b with the two-body chiral N^{3}LO interaction of Ref. [9] with the regulator parameter $\Lambda = 450$ MeV (referred to as EM17), and without the Coulomb interaction. The variational character of Λ_b is

again confirmed and convergence at the 0.5 MeV level of the binding energy is reached for $\Lambda_{\mathrm{b}} \approx 2.5$ fm^{-1}. With this value of Λ_{b}, the charge radius is converged at the 1% level. As expected, Λ_{b} is of the order of the interaction momentum scale $\Lambda_{NN} = \frac{\Lambda}{\hbar c} \approx 2.25$ fm^{-1}.

TABLE II

Hartree–Fock binding energy and charge radius of ^{16}O as a function of Λ_{b} with the EM17 interaction of Ref. [9] and using $L = 12.5$ fm.

Λ_{b} [fm^{-1}]	2.0	2.5	3.0	3.5	4.0
E_{b} [MeV]	−35.602	−39.481	−39.892	−39.908	−39.917
r_{c} [fm]	3.499	3.350	3.329	3.329	3.328

In Table III, the dependence on the box size is examined for ^{16}O and ^{48}Cr nuclei.

TABLE III

Variation of binding energy E_{b} (in MeV) and nuclear charge radius r_{c} (in fm) with the box size L (in fm). These calculations are performed with the EM17 interaction and without the Coulomb interaction, using $\Lambda_{\mathrm{b}} = 2.5$ fm^{-1}.

Nucleus	L	10.0	12.5	15.0	15.5	17.5
^{16}O	E_{b}	−41.073	−39.481	−39.516		−39.415
	r_{c}	3.378	3.350	3.335		3.338
^{48}Cr	E_{b}	−347.890	−335.634		−337.720	−337.010
	r_{c}	3.844	3.841		3.817	3.823

In the ^{48}Cr nucleus, the binding energy and the charge radius are well converged with a larger box size of about 15.5 fm than in ^{16}O, which is again about 4 to 5 times the charge radius.

The results of Tables II and III indicate that the EM17 interaction should be renormalized if one wants to be closer to experimental data at the Hartree–Fock approximation. In this work, as we aim at studying the behavior of the Hartree–Fock solutions with the confined plane-wave basis parameters, we transform the EM17 interaction into a low-momentum interaction by the Similarity Transformation Renormalization (SRG) approach [10] using a block-diagonal generator in the two-body sector with a sharp decoupling momentum of 2.0 fm^{-1}. We thus neglect the induced three-body interaction. Moreover, we neglect the matrix elements of the transformed potential between relative momenta larger than the decoupling momentum. In the following, we will refer to this renormalized interaction as

EM17+SRG(2.0). This choice allows us to use the single-particle momentum cutoff $\Lambda_{\rm b} = 2.0$ fm^{-1} and to reach heavier nuclei. Table IV shows the binding energy, charge radius and deformation quantities (axial quadrupole moment and the standard β_2 parameter) calculated with the EM17+SRG(2.0) interaction and without the Coulomb interaction in ^{16}O, ^{48}Cr and ^{98}Sr. In the ^{98}Sr nucleus, a reasonable convergence of all considered observables is expected with a box size of about 20 fm.

TABLE IV

Binding energy, charge radius and deformation quantities in the Hartree–Fock solutions obtained with the block-diagonal evolved EM17+SRG(2.0) interaction and, accordingly, $\Lambda_{\rm b} = 2.0$ fm^{-1}.

Nucleus	L	12.5	15.0	17.5	20.0
^{16}O	$E_{\rm b}$	−82.909	−82.179	−79.947	−79.704
	$r_{\rm c}$	3.230	3.247	3.290	3.301
^{48}Cr	$E_{\rm b}$	−518.131	−512.052	−493.088	−491.112
	$r_{\rm c}$	4.003	4.035	4.115	4.134
	Q_{20}	127.177	126.454	134.217	133.681
	β_2	0.27	0.27	0.27	0.27
^{98}Sr	$E_{\rm b}$		−1309.121	−1241.578	−1237.075
	$r_{\rm c}$		5.486	5.683	5.709
	Q_{20}		369.625	587.647	588.487
	β_2		0.26	0.39	0.38

To examine the dependence on the box size of the Hartree–Fock solutions including the Coulomb interaction, we add the direct Coulomb term in the Hartree–Fock calculation. As shown in Table V, the Coulomb energy basi-

TABLE V

Variation of the binding energy, direct Coulomb energy contribution and charge radius in the Hartree–Fock solution with the box size. The EM17+SRG(2.0) interaction is used and accordingly $\Lambda_{\rm b} = 2.0$ fm^{-1}.

Nucleus	L	12.5	15.0	17.5	20.0
^{16}O	$E_{\rm b}$	−63.027	−62.359	−60.367	
	$E_{\rm Coul}$	19.738	19.680	19.444	
	$r_{\rm c}$	3.263	3.278	3.320	
^{48}Cr	$E_{\rm b}$	−375.989	−370.544	−354.043	−352.312
	$E_{\rm Coul}$	141.190	140.572	138.164	137.923
	$r_{\rm c}$	4.038	4.068	4.147	4.165

cally remains unchanged and does not alter the previous conclusions about the box size, which has to be chosen at least of the order of 4 to 5 times the charge radius.

4.2. Full-fledged calculations

Based on this determination of the box size and the choice of the EM17+ SRG(2.0) interaction which permits us to fix the single-particle momentum truncation, the full Hartree–Fock calculations in which both direct and exchange Coulomb terms are included are performed in several deformed nuclei as shown in Tables VI and VII. In these calculations, the two-body kinetic-energy correction $\hat{K}_2$ is accounted for in a selfconsistent way. Its expectation value together with that of the one-body correction for comparison are displayed in Table VI.

TABLE VI

Binding energy E_b (in MeV), total Coulomb energy (in MeV), two- and one-body kinetic-energy corrections (in MeV), and nuclear charge radius r_c (in fm) in the Hartree–Fock solutions obtained with EM17+SRG(2.0) interaction. The basis parameters are $L = 17.5$ fm^{-1} and $\Lambda_\mathrm{b} = 2.0$ fm^{-1}.

Nucleus	E_b	E_Coul	$\langle\hat{K}_2\rangle$	$\langle\hat{K}_1\rangle$	r_c
^{16}O	−77.807	16.123	−7.813	22.045	3.264
^{24}Mg	−123.022	33.936	−10.552	24.273	3.708
^{28}Si	−161.382	45.718	−11.800	25.276	3.784
^{48}Cr	−378.607	126.519	−16.037	28.653	4.135
^{98}Sr	−966.303	284.542	−21.056	31.825	5.706

TABLE VII

Standard deformation parameters β_2 and γ in the Hartree–Fock solutions of Table VI, compared with the β_2 values calculated with the Skyrme parametrization SIII in an axially symmetric Hartree–Fock solutions.

Nucleus	β_2	γ	β_2 (SIII, axial)
^{24}Mg	0.39	5.6°	0.45
^{28}Si	−0.33	0	−0.30
^{32}S	0.21	15°	0.22
^{48}Cr	0.28	0	0.25
^{98}Sr	0.39	0	0.39

Although the calculated ground-state properties are in principle not meant to be compared with experimental data since we have neglected the three-body and higher contributions to the nuclear Hamiltonian (genuine and induced by the SRG transformation), we note that the deformation properties resulting from the transformed EM17+SRG(2.0) potential are found to be very close to those obtained with a phenomenological interaction SIII known to be in good agreement with experimental data. Moreover, we observe that the Coulomb energy in light nuclei such as ^{16}O, ^{24}Mg and ^{28}Si are comparable with the liquid-drop estimate $E_{\mathrm{Coul}} = a_{\mathrm{C}} Z^2/A^{1/3}$ with $a_{\mathrm{C}} = 0.7$ MeV. In the heavier nucleus ^{98}Sr, a larger deviation is found. Finally the two-body kinetic-energy correction is found to compensate of the order of 50% of the one-body kinetic-energy correction and steadily increases with the mass number as reported in Ref. [5].

5. Conclusions and perspectives

The Hartree–Fock approximation has been implemented in momentum space using a basis of plane waves confined in a cube. This basis is characterized by two parameters, the box size and a momentum cutoff, and is invariant under the full octahedral group with time-reversal symmetry. We have shown that this basis allows to represent very simply and economically matrix elements of a general nuclear two-body interaction through its momentum representation in the center-of-mass frame. In particular, no transformation coefficients such as Moshinky coefficients in the harmonic-oscillator representation or vector brackets in partial-wave representations are required. This advantage has been shown to also hold for the Coulomb interaction treated exactly. Moreover, we have chosen a self-consistent-symmetry group generated by intrinsic parity, z-signature and time-y-signature operators because it allows to describe triaxial shapes of nuclei in states that potentially break the time-reversal symmetry at the mean-field level with two quantum numbers (instead of one if the full dihedral double group with time-reversal symmetry is considered).

The study of the convergence of Hartree–Fock solutions with the basis parameters show that, on the one hand, the single-particle momentum cutoff has to be chosen at most as large as the relative-momentum cutoff scale in the nuclear interaction, on the other hand, the box size only depends on the nuclear radius. These conclusions are not altered by the presence of the Coulomb interaction. Finally, despite expected large discrepancies with experiment of binding energy and charge radius calculated at the Hartree–Fock level with only the two-body part of the interaction, good agreement is found for deformation properties.

Two obvious but challenging extensions of the present work are, on the one hand, the inclusion of three-body interactions (genuine and induced by the SRG transformation), on the other hand, the treatment of beyond-mean-field correlations. Moreover, our SRG-transformed Hamiltonians include only the nuclear part of the two-body interaction, so to be consistent, the Coulomb interaction should also be renormalized.

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