Operator overlaps in harmonic oscillator bases with different oscillator lengths

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A recently developed formalism is used to carry out generator coordinate method calculations using a set of Hartree-Fock-Bogoliubov wave functions, where each of the members of the set can be expanded in an arbitrary basis. In this paper it is assumed that the HFB wave functions are expanded in harmonic oscillator (HO) bases with different oscillator lengths. General expressions to compute the required matrix elements of arbitrary operators are given. The application of the present formalism to the case of fission is illustrated with an example.

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I. INTRODUCTION

Based on previous results published in Ref. [1], I developed in a recent publication [2] (denoted by I in the following) a formulation of the generalized Wick's theorem to compute overlaps between Hartree-Fock-Bogoliubov (HFB) wave functions expressed in different bases not connected by unitary transformations. In this paper, I apply the formalism to the common situation where one deals with two finite harmonic oscillator (HO) bases with different oscillator lengths. The present results could be of interest to carry out generator coordinate method (GCM) calculations and/or symmetry restoration [3–6] in fission; see [7,8] for a recent review and for a recent application. In fission one has to consider a set of HFB wave functions usually labeled in terms of the axial quadrupole moment $|\phi(q_{20})\rangle$ to study fission dynamics. The set of HFB states $|\phi(q_{20})\rangle$ span a large and rich set of nuclear shapes (from deformed ground states to configurations with a thin neck ending up finally in scission configurations) and therefore the oscillator lengths of the HO bases used have to adapt to the corresponding shape to reduce/optimize basis size. Typically, the oscillator lengths for each quadrupole moment are determined by minimizing the HFB energy, and the range of values obtained in a typical fission path can be rather large. As a consequence of the different oscillator lengths used for each q_{20} value, the bases used to express the corresponding HFB wave functions are not connected by unitary transformations (as a consequence of being finite dimensional). Therefore calculation of norm and Hamiltonian overlaps between the different configurations cannot be carried out with the traditional formulas [9,10] as they assume bases connected by unitary transformation, and therefore a generalization of Wick's theorem for overlaps between general HFB states is required. At this point it has to be mentioned that the evaluation of overlaps between Slater determinants [11] is properly handled even if the bases are not connected by unitary transformation. The most straightforward solution to this problem would be to use a common basis (with the same oscillator lengths) for all the HFB states in the fission path, but this solution demands huge harmonic oscillator bases and huge computational resources. At this point the reader might also wonder if it would not be better to use n unique, large enough basis for all the relevant HFB states, as is usually done in calculations in the mesh. This alternative is, however, impractical for all kind of interactions except for those of zero range with trivial local exchange terms. In order to find a practical solution to the above problems a generalization of the method used in [9,10] was formulated in Ref. [1]. The solution to all these problems relies on the formal extension of the original bases to make them complete and therefore unitarily connected. The basis states to be added come with zero occupancy. This approach has been pursued in Refs. [12,13] for unitary transformations and in Ref. [1] for general canonical ones. Years later, the Pfaffian formula for the proper calculation of the norm overlaps, including their sign [14,15], was subsequently generalized to consider different bases [16]. The inconvenience of the formulation of Ref. [1] is that additional considerations are required to come to the final formulas. Recently, in Ref. [2], I reformulated the work of Ref. [1] to simplify the expressions for the contractions entering the Hamiltonian and other operators' overlaps. The main advantage of the new formulation is that now it becomes evident that the operator's overlap can be obtained in terms of what is usually refereed to as "intrinsic quantities" (i.e., quantities that can be solely computed within the given finite bases). In this paper, I apply the formalism to the above mentioned situation of HO bases with different oscillator lengths. The required overlap matrix between the two HO bases with different lengths is explicitly built as well as its lower upper (LU) decomposition that plays a central role in the final expressions of Ref. [2]. The main

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application of the present formulation is to carry out GCM calculations or restore spatial symmetries in a fission framework. The new formulas could also be used to provide a more robust and precise formulation of the time dependent GCM. This will definitely help to improve our understanding of fission fragment properties and fission dynamics.

II. THE GENERALIZED WICK THEOREM FOR ARBITRARY BASIS

Recently [2], a convenient formalism to evaluate the overlap of general multi-body operators between arbitrary HFB wave functions

$$\frac{\langle\phi_0|\hat{O}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} \tag{1}$$

was laid down. In it, each of the HFB states entering the overlap are expanded in different bases not connected by unitary transformations (i.e., not expanding the same subspace of the whole Hilbert space). First, I establish the notation and then present the main results. The bases and associated creation operators are denoted by $\mathcal{B}_0 = \{c^\dagger_{0,k}, k = 1, \ldots, N_0\}$ in the case of $|\phi_0\rangle$ and $\mathcal{B}_1 = \{c^\dagger_{1,k}, k = 1, \ldots, N_1\}$ in the case of $|\phi_1\rangle$. Both bases satisfy canonical fermion antcommutation relations (CAR), i.e., $\{c^\dagger_{i,k}, c_{i,k'}\} = \delta_{kk'}$, and are connected by an overlap matrix $\{c^\dagger_{0,k}, c_{1,l}\} = {}_0\langle k|l\rangle_1 = \mathcal{R}_{kl}$. For simplicity, I assume in the following $N_0 = N_1 = N$, but note that the most general case can be easily accommodated in the formalism. One can also introduce the complement of the two bases $\bar{\mathcal{B}}_0 = \{c^\dagger_{0,k}, k = N+1, \ldots, \infty\}$ and $\bar{\mathcal{B}}_1 = \{c^\dagger_{1,k}, k = N+1, \ldots, \infty\}$ such that $\mathcal{B}_0 \cup \bar{\mathcal{B}}_0 = \{c^\dagger_{0,k}\}^\infty$ and $\mathcal{B}_1 \cup \bar{\mathcal{B}}_1 = \{c^\dagger_{1,k}\}^\infty$ expand the whole separable Hilbert space and therefore represent bases connected by a unitary (infinite dimensional) transformation matrix R (not to be confused with $\mathcal{R}$). Let me also introduce the quasiparticle annihilation operators $\alpha_{i\mu}$ $(i = 0, 1)$, which annihilate $|\phi_i\rangle$. They are written in terms of the complete bases $\{c^\dagger_{i,k}\}^\infty$ through the standard definition

$$\alpha_{i\mu} = \sum_k (U^*_i)_{k\mu} c_{i,k} + (V^*_i)_{k\mu} c^\dagger_{i,k}.$$

The Bogoliubov amplitudes U_i and V_i have a block structure,

$$V_i = \begin{pmatrix} \bar{V}_i & 0 \\ 0 & 0 \end{pmatrix}, \qquad U_i = \begin{pmatrix} \bar{U}_i & 0 \\ 0 & d_i \end{pmatrix},$$

where $\bar{V}_i$ and $\bar{U}_i$ are the $N \times N$ matrices characterizing $|\phi_i\rangle$. In this way, the set of N quasiparticle operators $\alpha_{i\mu}$ with $\mu = 1, \ldots, N$, correspond to the quasiparticle operators expanded in the truncated bases $\mathcal{B}_i$. The d_i are arbitrary unitary matrices that play no role in the final expressions. It is also convenient to express the unitary matrix R connecting $\mathcal{B}_0 \cup \bar{\mathcal{B}}_0$ with $\mathcal{B}_1 \cup \bar{\mathcal{B}}_1$ as a block matrix,

$$R = \begin{pmatrix} \mathcal{R} & \mathcal{S} \\ \mathcal{T} & \mathcal{U} \end{pmatrix}.$$

The matrix R is just the representation of the unitary operator $\hat{\mathcal{T}}_{01}$ connecting the two complete bases $\hat{\mathcal{T}}_{01} c^\dagger_{0,k} \hat{\mathcal{T}}^\dagger_{01} = c^\dagger_{1,k}$ whereas $\mathcal{R}$ is the restriction of this operator to the bases $\mathcal{B}_0$ and $\mathcal{B}_1$. In the present case, where one is dealing with HO bases differing in their oscillator lengths, $\hat{\mathcal{T}}_{01}$ is just the dilatation operator. As discussed in Appendix A, it is the exponential of a one-body operator. As shown in Ref. [2], the calculation of the overlap of Eq. (1) simplifies enormously if the operator $\hat{O}$ is written in second quantization form in terms of both bases $\{c^\dagger_{0,k}\}^\infty$ and $\{c^\dagger_{1,k}\}^\infty$. One-body operators are expressed in the form

$$\hat{O} = \sum_{kl} O^{01}_{kl} c^\dagger_{0,k} c_{1,l} \tag{2}$$

with

$$O^{01}_{kl} = {}_0\langle k|\hat{O}|l\rangle_1.$$

In the same way a two-body operator will be expressed as

$$\hat{O} = \frac{1}{4} \sum_{k_1 k_2 l_1 l_2} \tilde{v}^{01}_{k_1 k_2 l_1 l_2} c^\dagger_{0k_1} c^\dagger_{0,k_2} c_{1,l_2} c_{1,l_1}, \tag{3}$$

where the antisymmetrized two body matrix element is given by $\tilde{v}^{01}_{k_1 k_2 l_1 l_2} = v^{01}_{k_1 k_2 l_1 l_2} - v^{01}_{k_1 k_2 l_2 l_1}$, and $v^{01}_{k_1 k_2 l_2 l_1} = {}_0\langle k_1 k_2|\hat{v}|l_1 l_2\rangle_1$ are the interaction's matrix elements. The extension to higher order operators is straightforward. The sums in Eqs. (2) and (3) extend over the complete bases $\{c^\dagger_{0,k}\}^\infty$ or $\{c^\dagger_{1,k}\}^\infty$ to faithfully represent the operators. As shown in I, the overlaps of those operators can be obtained by using the standard rules of Wick's theorem but using the elementary contractions

$$\rho^{01}_{lk} = \frac{\langle\phi_0|c^\dagger_{0,k} c_{1,l}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \begin{cases} \left[\bar{V}^*_1 A^{-1} \bar{V}^T_0\right]_{lk}, & l \subset \mathcal{B}_0, k \subset \mathcal{B}_1, \\ 0, & \text{otherwise}, \end{cases} \tag{4}$$

$$\bar{\kappa}^{01}_{k_1 k_2} = \frac{\langle\phi_0|c^\dagger_{0,k_1} c^\dagger_{0,k_2}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \begin{cases} -\left[(\mathcal{R}^T)^{-1} \bar{U}^*_1 A^{-1} \bar{V}^T_0\right]_{k_1 k_2}, & k_1 \subset \mathcal{B}_0, k_2 \subset \mathcal{B}_0, \\ 0, & \text{otherwise}, \end{cases} \tag{5}$$

$$\kappa^{10}_{l_1 l_2} = \frac{\langle\phi_0|c_{1,l_1} c_{1,l_2}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \begin{cases} \left[\bar{V}^*_1 A^{-1} \bar{U}^T_0 (\mathcal{R}^T)^{-1}\right]_{l_1 l_2}, & l_1 \subset \mathcal{B}_1, l_2 \subset \mathcal{B}_1, \\ 0, & \text{otherwise}, \end{cases} \tag{6}$$

and therefore all the indices in the sums are restricted to the subspace spanned by $\mathcal{B}_0$ or $\mathcal{B}_1$. Although not obvious from the expressions in the right-hand side of Eqs. (5) and (6) the quantities $\bar{\kappa}^{01}_{k_1 k_2}$ and $\kappa^{10}_{l_2 l_1}$ are skew-symmetric matrices. In the above expressions, the matrix A is given by

$$A = \bar{U}^T_0 (\mathcal{R}^T)^{-1} \bar{U}^*_1 + \bar{V}^T_0 \mathcal{R} \bar{V}^*_1. \tag{7}$$

Using the above contractions the overlap of a one-body operator is given by

$$\frac{\langle\phi_0|\hat{O}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \sum_{k,l=1}^{N} O^{01}_{kl} \rho^{01}_{lk} = \mathrm{Tr}\left[O^{01} \rho^{01}\right], \tag{8}$$

whereas for a two-body matrix element one obtains

$$\frac{\langle\phi_0|\hat{O}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \frac{1}{4}\sum_{k_1,k_2,l_1,l_2=1}^{N} \tilde{v}^{01}_{k_1k_2l_1l_2}\big[\rho^{01}_{l_1k_1}\rho^{01}_{l_2k_2} - \rho^{01}_{l_1k_2}\rho^{01}_{l_2k_1} + \bar{\kappa}^{01}_{k_1k_2}\kappa^{10}_{l_2l_1}\big]. \tag{9}$$

Please remember that, contrary to the standard method, the matrices O^{01}_{kl}, ρ^{01}_{lk}, and $\tilde{v}^{01}_{k_1k_2l_1l_2}$ are not Hermitian but the matrices $\bar{\kappa}^{01}_{k_1k_2}$ and $\kappa^{10}_{l_1l_2}$ are still skew-symmetric. The overlap of the two HFB wave functions is

$$\langle\phi_0|\phi_1\rangle = \sqrt{\det A \det \mathcal{R}}. \tag{10}$$

In Ref. [2] a subsequent lower-upper (LU) decomposition of $\mathcal{R}$ was introduced,[1]

$$\mathcal{R} = L_0^* L_1^T, \tag{11}$$

where L_0 and L_1 are both lower triangular matrices. The decomposition introduces implicitly a biorthogonal basis $|k)_1 = \sum (L_1^T)^{-1}_{jk}|j\rangle_1$ and ${}_0(l| = \sum_0\langle i|(L_0^*)^{-1}_{li}$ such that ${}_0(l|k)_1 = \delta_{lk}$. The LU decomposition of the overlap matrix suggests the definitions

$$\tilde{U}_0 = (L_0^*)^{-1}\bar{U}_0 L_0^+, \quad \tilde{V}_0 = L_0^+\bar{V}_0 L_0^+, \tag{12}$$

$$\tilde{U}_1 = (L_1^*)^{-1}\bar{U}_1 L_1^+, \quad \tilde{V}_1 = L_1^+\bar{V}_1 L_1^+ \tag{13}$$

that turn out to be very useful to define handy quantities not depending explicitly on $\mathcal{R}$, for instance,

$$\tilde{A} = \tilde{U}_0^T\tilde{U}_1^* + \tilde{V}_0^T\tilde{V}_1^* = L_0^* A L_1^T. \tag{14}$$

The overlap is now written as

$$\langle\phi_0|\phi_1\rangle = \sqrt{\det \tilde{A}}. \tag{15}$$

It is also convenient to introduce the contractions

$$\tilde{\rho}^{01}_{lk} = \big[\tilde{V}_1^*\tilde{A}^{-1}\tilde{V}_0^T\big]_{lk} = L_1^T\rho^{01}L_0^*, \tag{16}$$

$$\tilde{\bar{\kappa}}^{01}_{k_1k_2} = -\big[\tilde{U}_1^*\tilde{A}^{-1}\tilde{V}_0^T\big]_{k_1k_2} = L_0^+\bar{\kappa}^{01}L_0^*, \tag{17}$$

$$\tilde{\kappa}^{10}_{l_1l_2} = \big[\tilde{V}_1^*\tilde{A}^{-1}\tilde{U}_0^T\big]_{l_1l_2} = L_1^T\kappa^{01}L_1. \tag{18}$$

Using them and the matrix elements $\tilde{O} = (L_0^*)^{-1}O^{01}(L_1^T)^{-1}$ one gets $\mathrm{Tr}(\tilde{O}\tilde{\rho}^{01})$ for the overlap of a one-body operator. Please note that $\tilde{O}_{lk}$ are the matrix elements of the operator $\hat{O}$ in the biorthogonal basis ${}_0(l|$ and $|k)_1$, i.e., $\tilde{O}_{lk} = {}_0(l|\hat{O}|k)_1 = \sum_{ij}(L_0^*)_{li_0^{-1}}\langle i|\hat{O}|j\rangle_1(L_1^T)^{-1}_{jk}$. Similar considerations apply to the overlap of two-body operators. Introducing the two-body matrix element in the biorthogonal basis $v^B_{ijkl} = {}_0(ij|\hat{v}|kl)_1$, related to v^{01}_{ijkl} by

$$v^B = (L_0^*)^{-1}(L_0^*)^{-1}v^{01}\big(L_1^T\big)^{-1}\big(L_1^T\big)^{-1},$$

one can define the HF potential $\tilde{\Gamma}^{01}_{ik} = \frac{1}{2}\sum \tilde{v}^B_{ijkl}\tilde{\rho}^{01}_{lj}$ and pairing field $\tilde{\Delta}^{01}_{ij} = \frac{1}{2}\sum \tilde{v}^B_{ijkl}\tilde{\kappa}^{01}_{kl}$ to write

$$\frac{\langle\phi_0|\hat{v}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \frac{1}{2}\mathrm{Tr}[\tilde{\Gamma}^{01}\tilde{\rho}^{01}] - \frac{1}{2}\mathrm{Tr}[\tilde{\Delta}^{01}\tilde{\bar{\kappa}}^{01}], \tag{19}$$

which is again the standard expression but defined in terms of Eqs. (16)–(18) and the definitions above. The advantage of the definitions in Eqs. (14), (16)–(18) is that they have exactly the same expression as the formulas available in the literature for complete bases but expressed in terms of the "tilde" U and V matrices of Eqs. (12) and (13). There is an additional advantage in the fact that $\tilde{A}$ is a "more balanced" matrix, being less affected by the near singular character of the overlap matrix $\mathcal{R}$.

III. APPLICATION TO HO BASES WITH DIFFERENT OSCILLATOR LENGTHS

To apply the above formalism to the case of HO bases with different oscillator lengths one just needs to compute the overlap matrix $\mathcal{R}_{kl} = {}_0\langle k|l\rangle_1$ and the overlap matrix elements $O^{01}_{kl} = {}_0\langle k|\hat{O}|l\rangle_1$ and ${}_0\langle k_1k_2|\hat{v}|l_1l_2\rangle_1$ for the harmonic oscillator bases with different oscillator lengths. To simplify the discussion, I will restrict to the case of a HO basis tensor product of one-dimensional (1D) states $\varphi_n(\vec{r}) = \prod_{i=1}^3\varphi_{n_i}(x_i,b_i)$ with $\varphi_{n_i}(x_i,b_i) = e^{-1/2x_i^2/b_i^2}\bar{\varphi}_{n_i}(x_i,b_i)$ the product of a Gaussian factor times a polynomial

$$\bar{\varphi}_{n_i}(x_i,b_i) = 1\Big/\sqrt{\sqrt{\pi}2^{n_i}n_i!b_i}\,H_{n_i}(x_i/b_i)$$

proportional to the Hermite polynomial H_n of degree n. As any polynomial of degree n can be written as a linear combination of $n+1$ polynomials of degree n or less, one can express $\bar{\varphi}_n(x,b_0)$ in terms of $\bar{\varphi}_n(x,b_1)$ by means of a finite-dimensional lower triangular transformation matrix $L_{nm}(q_{01})$ that depends on the ratio $q_{01} = b_1/b_0$ (see Appendix B):

$$\bar{\varphi}_n(x,b_0) = \sum_{m=0}^{n} L_{nm}(q_{01})\bar{\varphi}_m(x,b_1).$$

Due to the lower triangular structure of the matrix L, both its inverse and determinant can be obtained analytically (see Appendix B). It is now straightforward to compute the 1D overlaps

$$\begin{aligned}\mathcal{R}_{nm} &= \int dx\,\varphi_n^*(x,b_0)\varphi_m(x,b_1)\\ &= \int dx\,e^{-\frac{x^2}{B^2}}\bar{\varphi}_n^*(x,b_0)\bar{\varphi}_m(x,b_1)\\ &= \sum_r L^*_{nr}(q_0)L_{mr}(q_1),\end{aligned}$$

where the new oscillator length B is given by

$$1/B^2 = \tfrac{1}{2}\big(1/b_0^2 + 1/b_1^2\big) \tag{20}$$

and one has introduced the parameters $q_0 = B/b_0$ and $q_1 = B/b_1$. The matrices $L(q_i)$ are the ones transforming $\bar{\varphi}_m(x,b_i)$ into $\bar{\varphi}_m(x,B)$. The full overlap matrix is then given by

$$\mathcal{R}_{nm} = {}_0\langle n|m\rangle_1 = (L^*(\mathbf{q}_0)L^T(\mathbf{q}_1))_{nm} \tag{21}$$

[1] According to theorem 3.5.7 of [17] any nonsingular matrix A has a LU decomposition $A = PLU$ where P is a permutation matrix, and L (U) lower (upper) triangular nonsingular matrices. In the present development, the permutation matrix is omitted for simplicity as it is not required, but it can be easily considered in other cases.

with

$$L_{nm}(\mathbf{q}_0) = L_{n_x m_x}(q_{0x}) L_{n_y m_y}(q_{0y}) L_{n_z m_z}(q_{0z}). \tag{22}$$

It is obvious that the matrices $L(\mathbf{q}_i)$ have to be identified with the L_i introduced in Eq. (11). The matrix $L_{nm}(\mathbf{q}_0)$ can be also arranged as a triangular matrix if one takes the standard ordering $n = (n_x, n_y, n_z)$ with $n_x = 0, \ldots, N_x$, $n_y = 0, \ldots, N_y(n_x)$, and $n_z = 0, \ldots, N_z(n_x, n_y)$. With this ordering the inverse matrix $L^{-1}_{nm}(\mathbf{q}_0)$ can also be written in analytical form in terms of the inverse of the 1D quantities given in Appendix B,

$$L^{-1}_{nm}(\mathbf{q}_0) = L^{-1}_{n_x m_x}(q_{0x}) L^{-1}_{n_y m_y}(q_{0y}) L^{-1}_{n_z m_z}(q_{0z}). \tag{23}$$

The determinant of $\mathcal{R}$ is given by the product of the determinant of two lower triangular matrices

$$\det \mathcal{R} = (\det[L(\mathbf{q}_0)])^* \det[L(\mathbf{q}_1)].$$

Given the lower triangular structure of the $L(\mathbf{q}_i)$ matrices, their determinant is just the product of the elements in the diagonal $\det[L(\mathbf{q}_i)] = \prod'_{n_x,n_y,n_z} q_{ix}^{n_x+1/2} q_{iy}^{n_y+1/2} q_{iz}^{n_z+1/2}$, where the product is restricted to those values of n_x, n_y, and n_z compatible with the definition of the basis (typically, some energy condition, $\sum_{n_x,n_y,n_z} \hbar\omega_x(n_x + 1/2) + \hbar\omega_y(n_y + 1/2) + \hbar\omega_z(n_z + 1/2) < E_0$). The explicit form of the LU decomposition of the 1D $\mathcal{R}$ immediately suggests the introduction of the biorthogonal states

$$\langle x|m\rangle_1 = e^{-\frac{x^2}{2B^2}} \bar{\varphi}_m(x, B) = e^{-\frac{x^2}{2B^2}} \sum_{m'} L^{-1}_{mm'}(q_1) \bar{\varphi}_{m'}(x, b_1) \tag{24}$$

and

$${}_0\langle n|x\rangle = e^{-\frac{x^2}{2B^2}} \bar{\varphi}^*_n(x, B) = e^{-\frac{x^2}{2B^2}} \sum_{n'} L^{*-1}_{nn'}(q_0) \bar{\varphi}^*_{n'}(x, b_0) \tag{25}$$

such that ${}_0\langle n|m\rangle_1 = \delta_{nm}$. Clearly, bras and kets of the biorthogonal states turn out to be connected by Hermitian conjugation and therefore they form a unique set of orthogonal states thanks to the special properties of the HO states. This unique set is just a set of HO wave functions with oscillator length B.

The matrix elements of one-body momentum-independent operators $\hat{O}$ can be expressed in terms of the matrix elements computed with the orthogonal basis with oscillator length $\boldsymbol{B} = (B_x, B_y, B_z)$:

$${}_0\langle n|\hat{O}|m\rangle_1 = (L^*(\mathbf{q}_0) O_{\boldsymbol{B}} L^T(\mathbf{q}_1))_{nm}. \tag{26}$$

Here $O_{\boldsymbol{B}}$ is the matrix of the matrix elements of $\hat{O}$ computed with the HO basis with lengths $\boldsymbol{B}$. In the case of two-body momentum independent operators like the central or Coulomb potentials the generalization is again straightforward:

$${}_0\langle nm|\hat{v}|pq\rangle_1 = \sum_{rstu} L^*(\mathbf{q}_0)_{nr} L^*(\mathbf{q}_0)_{ms} \langle rs|\hat{v}|tu\rangle_{\boldsymbol{B}} \tag{27}$$

$$L(\mathbf{q}_1)_{pt} L(\mathbf{q}_1)_{qu}, \tag{28}$$

where $\langle rs|\hat{v}|tu\rangle_{\boldsymbol{B}}$ are the matrix elements of the two-body potential computed with HO states with length $\boldsymbol{B}$.

For the evaluation of momentum dependent operators like the kinetic energy or the spin-orbit potential the easiest way is to use recursion relations like

$$\frac{\partial}{\partial x}\widetilde{\varphi}_n(x) = \frac{1}{\sqrt{2}B}\left(q_0^2\sqrt{n}\widetilde{\varphi}_{n-1}(x) - q_1^2\sqrt{n+1}\widetilde{\varphi}_{n+1}(x)\right) \tag{29}$$

and

$$\begin{aligned}\frac{\partial^2}{\partial x^2}\widetilde{\varphi}_n(x) = \frac{1}{2B^2}\big(&q_0^4\sqrt{n(n-1)}\widetilde{\varphi}_{n-2}(x) \\ &- q_0^2 q_1^2(2n+1)\widetilde{\varphi}_n(x) \\ &+ q_1^4\sqrt{(n+1)(n+2)}\widetilde{\varphi}_{n+2}(x)\big),\end{aligned} \tag{30}$$

where $\widetilde{\varphi}_n(x) = e^{-\frac{x^2}{2b_1^2}} \bar{\varphi}_n(x, B)$. For instance, the matrix elements of the one-body kinetic energy operator are given by

$${}_0\langle n|\hat{T}|m\rangle_1 = (L^*(\mathbf{q}_0) T_{\boldsymbol{B}} L^T(\mathbf{q}_1))_{nm},$$

where the matrix elements $T_{\boldsymbol{B}}$ are computed in the traditional way, using HO with oscillator lengths $\boldsymbol{B}$ but using the recursion relations of Eqs. (29) and (30) instead of the traditional ones. The same recursion relations can be used in the evaluation of the matrix elements of the two-body spin-orbit potential. Note that the corresponding formulas for the two-dimensional HO wave functions often used in axially symmetric codes can be found in Appendix C.

In the application of the present formalism to the case where density dependent interactions like Skyrme or Gogny are used one has to use a prescription for the density dependent term [12,18–20]. The prescription used is the so-called overlap prescription that amounts to using the density

$$\rho_{\rm ov}(\vec{r}) = \frac{\langle\phi_0|\hat{\rho}(\vec{r})|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \sum_{k,l=1}^{N} \varphi^*_k(\vec{r}; b_0)\varphi_l(\vec{r}; b_1)\rho^{01}_{lk}$$

in the density dependent term of the interaction.

As mentioned in the previous section [Eqs. (12) and (13)] it is convenient to introduce the matrices

$$\tilde{V}_i = L^+(\mathbf{q}_i)\bar{V}_i L(\mathbf{q}_i), \tag{31}$$

$$\tilde{U}_i = [L^*(\mathbf{q}_i)]^{-1}\bar{U}_i L(\mathbf{q}_i), \tag{32}$$

and

$$\tilde{A} = \tilde{U}_0^T\tilde{U}_1^* + \tilde{V}_0^T\tilde{V}_1^* = L^T(\mathbf{q}_0) A L^*(\mathbf{q}_1). \tag{33}$$

They allow one to simplify the expression of the overlap to

$$\langle\phi_0|\phi_1\rangle = \sqrt{\det\tilde{A}}. \tag{34}$$

This formula is not only simpler than the original one but allows one to avoid a common problem in typical applications: the exceedingly large or small values of $\det L(\mathbf{q})$ can overflow or underflow the floating point computer representation of real numbers. This problem is discussed in the following section. Using the definitions of Eqs. (31) and (32) one can also introduce the density matrix contraction of Eq. (16) to express the overlap of one-body operators in Eq. (8) as

$$\frac{\langle\phi_0|\hat{O}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \sum_{k,l=1}^{N} O^{01}_{kl}\rho^{01}_{lk} = \mathrm{Tr}[O_{\boldsymbol{B}}\tilde{\rho}^{01}], \tag{35}$$

given in terms of the matrix elements of the operator in the HO basis with oscillator lengths $\boldsymbol{B} = (B_x, B_y, B_z)$, i.e., there

is no need to consider additional formulas for matrix element overlap. The same applies to the calculation of two-body terms like the overlap of the potential energy, Eq. (9). so that one can write finally

$$\frac{\langle\phi_0|\hat{v}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \frac{1}{2}\mathrm{Tr}[\tilde{\Gamma}^{01}\tilde{\rho}^{01}] - \frac{1}{2}\mathrm{Tr}[\tilde{\Delta}^{01}\tilde{\kappa}^{01}] \tag{36}$$

with the HF potential

$$\tilde{\Gamma}^{01}_{ik} = \frac{1}{2}\sum \tilde{v}^{\boldsymbol{B}}_{ijkl}\tilde{\rho}^{01}_{lj} \tag{37}$$

and pairing field

$$\tilde{\Delta}^{01}_{ij} = \frac{1}{2}\sum \tilde{v}^{\boldsymbol{B}}_{ijkl}\tilde{\kappa}^{01}_{kl} \tag{38}$$

computed with matrix elements of the potential in the HO basis with lengths $\boldsymbol{B}$ [except for the momentum dependent terms of the potential where, additionally, one has to use the modified recursion relations of Eqs. (29) and (30)]. For the spatial overlap density one finally obtains

$$\rho_{\mathrm{ov}}(\vec{r}) = \sum_{k,l=1}^{N} \varphi^*_k(\vec{r};B)\varphi_l(\vec{r};B)\tilde{\rho}^{01}_{lk}.$$

To summarize this section, the calculation of overlaps of operators between HFB states expressed in HO basis with different oscillator lengths involves

(1) Computing matrix elements of the operators with a set of HO functions with oscillator length parameters $\boldsymbol{B}$ given by Eq. (20).
(2) Computing the $\tilde{U}_i$ and $\tilde{V}_i$ Bogoliubov amplitudes (31) and (32) and $\tilde{A}$ in Eq. (33).
(3) Computing the density matrix and pairing tensor contractions of Eqs. (16)–(18).
(4) Evaluating the HF potential (37) and pairing field (38).
(5) Evaluate overlaps for one-body operator (35) and two-body operator (36).

Please note that Eqs. (33), (16)–(18) have the traditional form but in terms of $\tilde{U}_i$ and $\tilde{V}_i$ Bogoliubov amplitudes (31) and (32). Therefore, the modifications required to implement the formalism described in an existing computer code are minimal and easy to implement.

IV. APPLICATION OF THE METHOD

In this section the formalism will be used to compute the overlaps between the members of the set of wave functions $|\phi(q_{20})\rangle$ entering the fission path of the nucleus ^{238}Pu. Traditionally, those wave functions are computed in a HO basis with oscillator lengths tailored to the deformation q_{20} and obtained by minimizing the HFB energy as a function of the oscillator lengths. The results will be compared to the ones obtained by a blind application of the standard formulas. To motivate the discussion, I display in Fig. 1 the potential energy surface (PES) obtained as a function of the axial quadrupole moment q_{20} with the Gogny force D1M* [21,22]. In the calculation I use an axial HO basis with 18 shells in the perpendicular direction and 27 shells in the z direction.

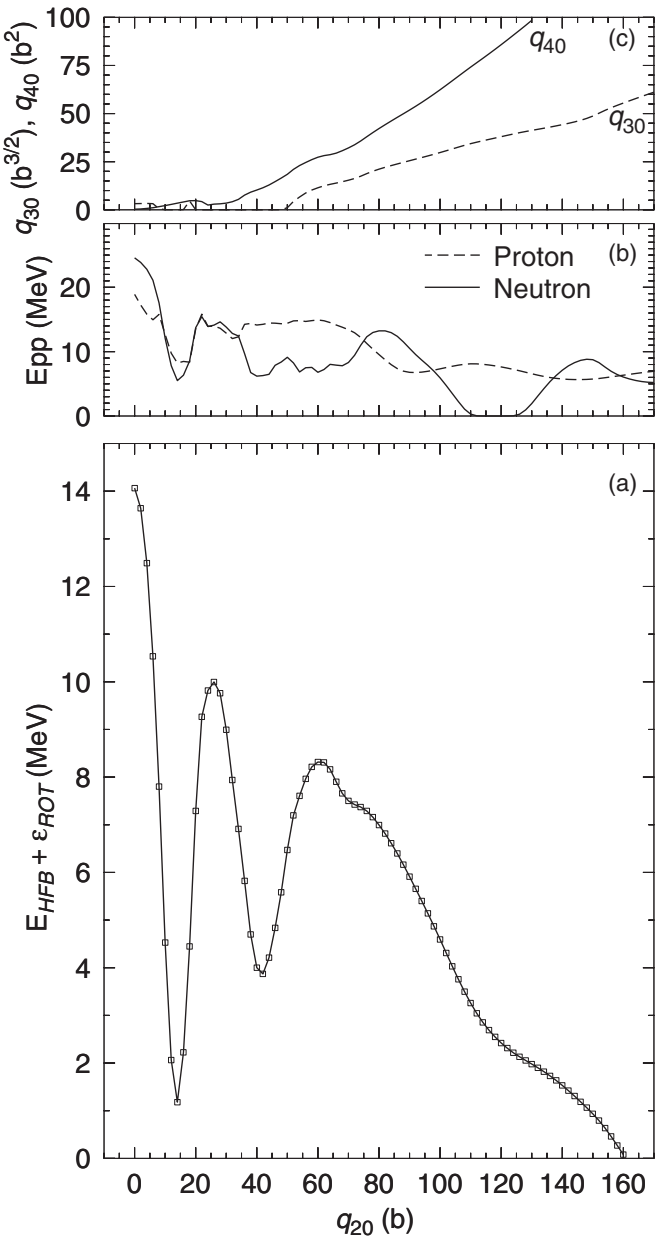

FIG. 1. In the lower panel, the potential energy surface (including the rotational energy correction) of ^{238}Pu is depicted as a function of the quadrupole moment q_{20} (in barns). The energy has been shifted by 1800 MeV. In the middle panel the particle-particle (pairing) correlation energies are shown for both protons and neutrons. In the upper panel, the octupole q_{30} and hexadecapole q_{40} moments are given as a function of q_{20}. The multipole moments are defined, for instance, in [23].

In Fig. 1, apart from the HFB energy plus the rotational correction [panel (a)], other relevant quantities like the particle-particle pairing energies for protons and neutrons [panel (b)] and the octupole and hexadecapole moments [panel (c)] are shown. One is dealing with a standard actinide with a deformed ground state, a fission isomer at $q_{20} = 44$ b,

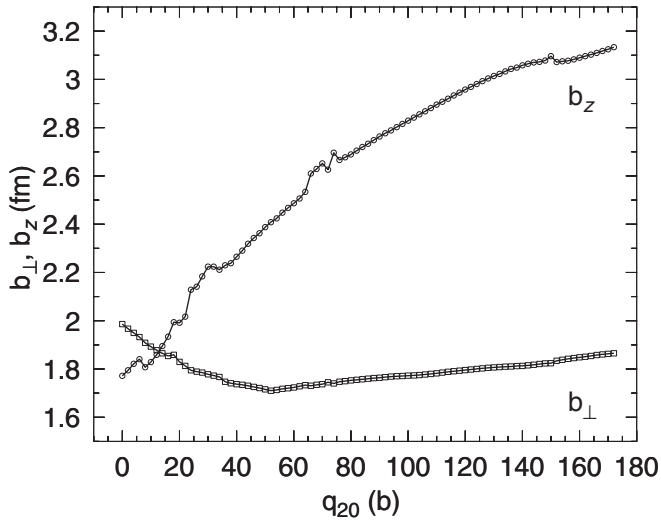

FIG. 2. Oscillator lengths $b_\perp$ and b_z for each HFB configuration $|\phi(q_{20})\rangle$.

and two barriers (inner and outer). At $q_{20} = 50$ b, the HFB solution starts breaking reflection symmetry and a nonzero octupole moment develops.

The oscillator lengths $b_\perp$ and b_z obtained by minimizing the HFB energy for each value of the quadrupole moment q_{20} are depicted in Fig. 2. The abrupt changes observed at some q_{20} values are due to coexisting minima in the HFB energy $E_{\rm HFB}(q_{20})$ as a function of $b_\perp$ and b_z. I could have chosen the oscillator lengths as to obtain a smoother curve in Fig. 2, but I have preferred to leave it that way because this is the typical outcome of an automatized procedure. As shown in Fig. 2, b_z increases monotonically with q_{20} whereas $b_\perp$ remains roughly constant in the whole interval. It is also evident that there are large variations in b_z depending on the value of the quadrupole moment.

To illustrate the results obtained with the present formalism, I have chosen three emblematic values of q_{20}, namely 40, 80, and 120 b, and varied the corresponding optimal oscillator lengths by ± 0.05 fm to obtain different HFB solutions. Those solutions have roughly the same energy and other observables as the starting one, indicating that the HFB wave function is essentially the same in all the cases. However, as the oscillator length parameters have slightly changed, the HFB amplitudes must be slightly different to absorb the changes in the basis parameters. As a consequence, one expects the traditional formula for the overlap (i.e., the one not taking into account that the bases are different) to give values differing from 1. On the other hand, the formalism introduced here should provide an overlap close to 1. The results obtained are summarized in Table I. They clearly show how the traditional overlap formula is wrong whereas the present formalism provide the expected results, namely overlaps very close to 1.

To finalize this section, consider now the overlaps $\langle\phi(q_{20})|\phi(q_{20}^{(0)})\rangle$ with $q_{20}^{(0)} = 40$, 60, and 80 b as a function of q_{20}. They are plotted in logarithmic scale in Fig. 3 as a function of $(q_{20} - q_{20}^{(0)})^2$, motivated by the fact that in the Gaussian overlap approximation $\langle\phi(q_{20})|\phi(q_{20}^{(0)})\rangle \approx \exp[-\gamma(q_{20})(q_{20} - q_{20}^{(0)})^2]$. The exact overlaps computed with Eq. (34) are represented with a solid line whereas the wrong ones, computed with the Onishi-Yoshida formula [9], are plotted using dotted lines. There are several salient features worth mentioning. First, the overlaps given by the Onishi-Yoshida formula are almost always larger than the correct ones. The reason is that, as the oscillator lengths are adapted to the quadrupole moment, the basis is partially responsible for generating quadrupole deformation and therefore the Bogoliubov amplitudes of neighboring configurations change less than if the oscillator lengths of the basis were kept constant. The feature shows some exceptions in a limited q_{20} region in the $q_{20}^{(0)} = 60$ b case where the oscillator lengths as a function of q_{20} show a less smooth behavior than in the other cases. Second, the overlap decreases faster with Eq. (34) than with the Onishi-Yoshida formula except in a limited q_{20} range in the $q_{20}^{(0)} = 60$ b case. Third, in the $q_{20}^{(0)} = 60$ b case Eq. (34) provides far more smooth results than the Onishi-Yoshida formula, indicating that Eq. (34) is able to absorb the changes is the oscillator lengths taking place in this case. Fourth, the Gaussian overlap formula seems to be rather inaccurate in the $q_{20}^{(0)} = 40$ b and 60 b cases as the behaviors of the overlap in the given scales depart from the expected straight line. Finally, I briefly discuss the large and small values of $\det L_i$ found in the calculation of the overlaps. As a typical example, consider $q_{20}^{(0)} = 40$ b and $q_{20} = 60$ b. In this case, $\det L_0 = 1.88 \times 10^{186}$ and $\det L_1 = 6.81 \times 10^{-208}$, giving $\det \mathcal{R} = 1.28 \times 10^{-21}$.

TABLE I. Overlaps between different HFB solutions obtained with slightly different oscillator lengths. The optimal oscillator lengths $(b_\perp, b_z)$ are (1.75, 2.25), (1.75, 2.75), and (1.80,2.95) for $q_{20} = 40$, 80, and 120 b, respectively. The column denoted as "Trad." corresponds to the traditional calculation of the overlaps without taking into account the effect of the bases (Onishi-Yoshida formula [9]).

	$q_{20} = 40$ b			$q_{20} = 80$ b			$q_{20} = 120$ b		
Config.	$E_{\rm HFB}$	Eq. (34)	Trad.	$E_{\rm HFB}$	Eq. (34)	Trad.	$E_{\rm HFB}$	Eq. (34)	Trad.
Optimal	−1792.104	1.0	1.0	−1788.366	1.0	1.0	−1792.883	1.0	1.0
$b_z + 0.05$	−1792.040	0.999	0.721	−1788.317	0.999	0.747	−1792.841	0.999	0.766
$b_z + 0.10$	−1791.931	0.998	0.279	−1788.216	0.997	0.322	−1792.746	0.998	0.354
$b_z - 0.05$	−1792.064	0.998	0.709	−1788.324	0.999	0.735	−1792.841	0.999	0.755
$b_z - 0.10$	−1791.838	0.993	0.243	−1788.155	0.994	0.283	−1792.841	0.996	0.315
$b_\perp + 0.05$	−1792.099	0.999	0.820	−1788.360	0.999	0.830	−1792.873	0.999	0.803
$b_\perp - 0.05$	−1792.099	0.999	0.813	−1788.366	0.999	0.824	−1792.868	0.999	0.797

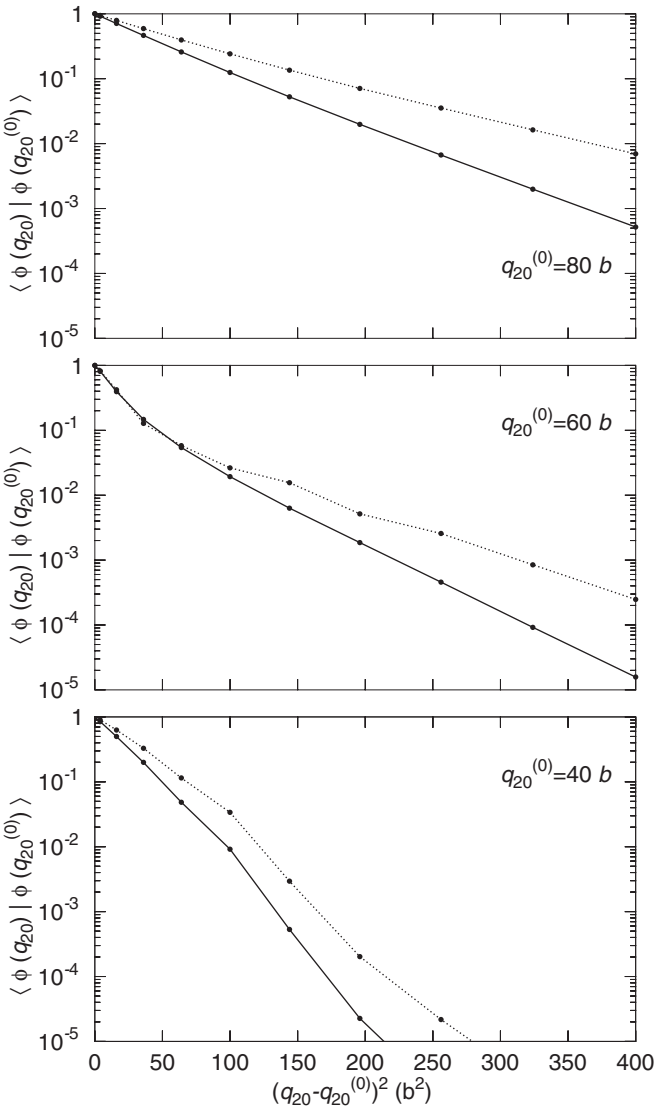

FIG. 3. Overlaps $\langle\phi(q_{20})|\phi(q_{20}^{(0)})\rangle$ for $q_{20} \geqslant q_{20}^{(0)}$ are plotted as a function of $(q_{20} - q_{20}^{(0)})^2$ for different representative values of $q_{20}^{(0)}$. Full lines are obtained with Eq. (34) and dotted ones obtained with the Onishi-Yoshida formula [9].

At $q_{20} = 64$ b, $\det \mathcal{R} = 1.2 \times 10^{-30}$, but the overlap for protons is still relatively relevant with a value of 2.03×10^{-4}. However, at $q_{20} = 66$ b, $\det L_1$ underflows the 64 bit floating point representation used in the calculations, and $\det \mathcal{R} = 0$ to machine accuracy. A bit further, at $q_{20} = 68$ b the determinant $\det L_0$ is the one that overflows and the computer value for $\det \mathcal{R}$ is undefined. However, using Eqs. (14) and (15) the evaluation of the overlap proceeds smoothly and, what is more important, unattended.

V. SUMMARY AND CONCLUSIONS

Formulas are given to compute correctly overlaps of operators between HFB states expressed in bases which are not unitarily equivalent. They allow for an efficient implementation of the GCM in cases where the relevant shapes involved are very different, like in fission, and require HO bases with very different values of the oscillator lengths. The present results open up the possibility of implementing the time dependent GCM to understand fission dynamics. The generalization to cases requiring symmetry restoration is straightforward and only requires the calculation of the corresponding overlap matrix between the elements of the bases.

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APPENDIX A: THE DILATATION OPERATOR

The dilatation operator in 1D, $\hat{\mathcal{T}}(a)$, satisfies $\langle x|\hat{\mathcal{T}}(a) = \langle ax|$, where $|x\rangle$ is an eigenstate of the position operator. Therefore, for an arbitrary state vector $|\Psi\rangle$, one has $\langle x|\hat{\mathcal{T}}(a)|\Psi\rangle = \Psi(ax)$. In one dimension, the operator is given by

$$\hat{\mathcal{T}}'(a) = e^{\tau x \partial_x}$$

with $a = e^{\tau}$. As it stands, the operator is not unitary as the exponent is not an anti-Hermitian operator. As can be easily checked, just adding $\tau/2$ to the exponent will do the trick. The unitary dilation operator is then given by

$$\hat{\mathcal{T}}(a) = e^{\tau(x\partial_x + \frac{1}{2})}.$$

With this definition $\hat{\mathcal{T}}(a)f(x) = e^{\tau/2} f(e^{\tau}x)$. The extra factor $\exp(\tau/2)$ is usually absorbed by the normalization constant, as is the case for the harmonic oscillator wave function

APPENDIX B: TRANSFORMATION COEFFICIENT L IN ONE DIMENSION

In this Appendix I establish the explicit expression of the L coefficients in the expansion of the restricted 1D HO wave functions

$$\bar{\varphi}_n(x, b_0) = \sum_{m=0}^{n} L_{nm}(q_{01}) \bar{\varphi}_m(x, b_1)$$

with $q_{01} = \frac{b_1}{b_0}$. They are given by

$$L_{nm}(q) = \Delta_{n,m} \frac{\left(\frac{n!}{m!}\right)^{1/2}}{2^{(n-m)/2}\left(\frac{n-m}{2}\right)!} (q^2 - 1)^{\frac{n-m}{2}} q^{m+1/2}, \qquad \text{(B1)}$$

where $\Delta_{n,m} = \frac{1}{2}[1 + (-)^{n+m}]$ is the "parity" Kronecker symbol. The L_{nm} also satisfy $L_{nm} = 0$ if $m > n$ due to the factorial in the denominator and therefore they are the matrix elements of a lower triangular matrix. The expression of Eq. (B1) is easily obtained by using the generating function of the Hermite polynomials

$$\sum_n \frac{t^n}{n!} H_n(x) = e^{2xt - t^2}.$$

The inverse of the 1D matrix L can be found by inspection:

$$L^{-1}_{mr}(q) = \Delta_{m,r}\frac{(-)^{\frac{m-r}{2}}\left(\frac{m!}{r!}\right)^{1/2}}{2^{(m-r)/2}\left(\frac{m-r}{2}\right)!}(q^2-1)^{\frac{m-r}{2}}q^{-(m+1/2)}. \quad \text{(B2)}$$

Due to the triangular form, the determinant of L can also be computed right away: assuming the dimension of the matrix is N (i.e., $m = 0, \ldots, N-1$),

$$\det L = \prod_{m=0}^{N-1} q^{m+1/2} = q^{N^2/2}$$

APPENDIX C: TRANSFORMATION COEFFICIENT L IN TWO DIMENSIONS

The generalization of the results of Appendix B to the two-dimensional case that one encounters in the harmonic oscillator basis with axial symmetry is straightforward. The 2D HO wave function is defined in terms of the $n_\perp$ and m quantum numbers as

$$\phi_{n_\perp m}(\vec{r}, b) = e^{-\frac{1}{2}r_\perp^2}\bar{\phi}_{n_\perp m}(\vec{r}, b)$$

with

$$\bar{\phi}_{n_\perp m}(\vec{r}, b) = \mathcal{N}_\perp\left(\frac{r_\perp}{b}\right)^{|m|}L^{|m|}_{n_\perp}\left(\frac{r_\perp^2}{b^2}\right)e^{im\varphi}$$

and $\mathcal{N}_\perp = \frac{1}{b\sqrt{\pi}}\left(\frac{n_\perp!}{(n_\perp+|m|)!}\right)^{1/2}$. The generating function is in this case

$$\exp\left(\frac{2\vec{r}\vec{t}}{b} - t^2\right) = \sum_{n_\perp m}\kappa^*_{n_\perp m}(\vec{t})\bar{\phi}_{n_\perp m}(\vec{r}, b),$$

where $\vec{t}$ is a two-dimensional vector and the coefficients in the linear combination are given by

$$\kappa^*_{n_\perp m}(\vec{t}) = (-)^{n_\perp}\frac{\sqrt{\pi}b}{(n_\perp!(n_\perp+|m|)!)^{1/2}}t_\perp^{2n_\perp+|m|}e^{-im\varphi_t}.$$

Expanding the identity

$$\exp\left(\frac{2\vec{r}\vec{t}}{b} - t^2\right) = \exp\left(\frac{2\vec{r}(q\vec{t})}{b'} - q^2t^2\right)\exp[(q^2-1)t^2]$$

in powers of $t_\perp$ and φ_t and equating equal powers in both sides, one obtains

$$\bar{\phi}_{n_\perp m}(\vec{r}, b) = \sum_{n'_\perp} L^{|m|}_{n_\perp n'_\perp}(q)\bar{\phi}_{n'_\perp m}(\vec{r}, b')$$

with

$$L^{|m|}_{n_\perp n'_\perp}(q) = q^{2n'_\perp+|m|+1}\frac{(1-q^2)^{n_\perp-n'_\perp}}{(n_\perp-n'_\perp)!}\left(\frac{n_\perp!(n_\perp+|m|)!}{n'_\perp!(n'_\perp+|m|)!}\right)^{1/2}$$

and $q = b'/b$. It is usually more convenient to express the quantum numbers in terms of $N = 2n_\perp + |m|$ and m. Using them, one obtains

$$L_{(N,m)(N',m')}(q) = \frac{\delta_{mm'}(-)^{\frac{N-N'}{2}}}{\left(\frac{(N-N')}{2}\right)!}\left(\frac{\left(\frac{N\pm m}{2}\right)!}{\left(\frac{N'\pm m'}{2}\right)!}\right)^{1/2} \times (1-q^2)^{\frac{N-N'}{2}}q^{(N'+1)}$$

and, for the inverse,

$$L^{-1}_{(N,m)(N',m')}(q) = \frac{\delta_{mm'}(-)^{\frac{N-N'}{2}}}{\left(\frac{(N-N')}{2}\right)!}\left(\frac{\left(\frac{N\pm m}{2}\right)!}{\left(\frac{N'\pm m'}{2}\right)!}\right)^{1/2} \times (1-q^2)^{\frac{N-N'}{2}}q^{-(N+1)},$$

as can be easily obtained by inspection. In the above formulas $(\frac{N\pm m}{2})! = (\frac{N-m}{2})!(\frac{N+m}{2})!$.

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