Letter

# Formulation of the generator coordinate method with arbitrary bases

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The existing formalism used to compute the operator overlaps necessary to carry out generator coordinate method calculations using a set of Hartree-Fock-Bogoliubov wave functions is generalized to the case where each of the HFB states are expanded in different arbitrary bases spanning different subspaces of the Hilbert space.

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The calculation of operator overlaps between general Hartree-Fock (HF or Slater) or Hartree-Fock-Bogoliubov (HFB) mean-field wave functions is a common task in many areas of physics like nuclear physics [1], condensed matter physics [1], or quantum chemistry [2]. It is required in the restoration of spontaneously broken (by the mean field) symmetries or in the consideration of fluctuations beyond the mean field in the context of the configuration interaction or the generator coordinate method [1,3–5]. In both cases, linear combinations of mean-field wave functions of the HF or HFB type are used to build a variational space. The set of HFB wave functions is usually chosen to explore the corner of the Hilbert space relevant to the physics to be described or it is dictated by the symmetry to be restored. The evaluation of the overlaps is greatly simplified by using the generalized Wick theorem (GWT) for general HFB states [6,7] or its equivalent for Slater determinants [8]. Generalizations to consider different peculiarities in the calculations of the overlaps have been developed over the years both at zero [9–13] or finite temperature [14–16]. The GWT implicitly assumes that all the quasiparticle operators of the Bogoliubov transformation are expanded in a common basis that is often taken as finite dimensional due to computational complexity reasons. However, in many practical applications the parameters of the basis (for instance, oscillator lengths in the harmonic oscillator basis case) to be used for each of the HFB states have different values or, in the context of symmetry restoration, the basis is not closed under the symmetry operation (for instance, an arbitrary translation of the HO basis). The most straightforward solution to this problem is to use a common basis (with the same oscillator lengths) for all the states of the HFB set or, in the case of symmetry restoration, a basis which is closed under the symmetry operation (HO basis with the same oscillator lengths along the three spatial directions in the case of rotations, a plane wave basis in the case of translations, etc.). However, if the use of a localized basis is required along with spatial translations, the only easy strategy is to use a very big basis and to carefully check the convergence of the results with basis size [17,18]. These simple strategies come at a cost; namely, they increase the basis size and, therefore, the computational complexity. The situation is specially delicate, for instance, in fission studies where the very broad range of nuclear shapes to be considered in the fission process makes it impractical to use a basis with equal oscillator lengths (in fact, all practitioners of fission using either one-center or two-center HO bases often use different, optimized basis parameters for each quadrupole moment defining the fission process) [19,20]. At this point the reader might wonder why not to do the calculation in the mesh. This solution is, however, impractical in general and it is only useful for zero-range interactions with trivial local exchange terms. In addition, one has to carefully consider [21] the assumptions and approximations required to implement the generators of the symmetry in the mesh. Therefore, the only viable solution to all the problems with noncomplete bases relies on the formal extension of the original basis to make it complete with the added states having zero occupancy. This approach has been pursued in Refs. [22,23] for unitary transformations and in Ref. [9] for general canonical transformations. However, in those references it is not clear whether one can compute the overlaps in terms of quantities defined in the starting, finite size, bases. The purpose of this paper is to extend the formalism of Ref. [9] to prove that the overlaps can always be obtained in terms of what I call intrinsic quantities (i.e., quantities that are defined solely in the given finite bases), and therefore, there is no need to refer to the complementary (often infinite-dimensional) subspace required to make the bases complete. In addition, by using the lower-upper (LU) decomposition of the overlap matrix between the elements of the bases, it will be possible to express all the different quantities in a more familiar form, facilitating the application of the obtained formulas. The application of the formalism to the use of harmonic oscillator wave functions with different oscillator lengths or the more general case involving rotated and translated basis is deferred to future publications.

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The goal of this paper is to evaluate the overlap of general multibody operators between arbitrary HFB wave functions,

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

where each of the HFB states are expanded in different bases not connected by unitary transformations (i.e., not expanding the same subspace of the whole Hilbert space). I denote the corresponding bases and associated creation operators as $\mathcal{B}_0 = \{c^\dagger_{0,k}, k = 1, \dots, N_0\}$ in the case of $|\phi_0\rangle$ and $\mathcal{B}_1 = \{c^\dagger_{1,k}, k = 1, \dots, N_1\}$ in the case of $|\phi_1\rangle$. It is implicitly assumed that fermion canonical anticommutation relations (CARs) are preserved among each basis set, i.e., $\{c_{i,k}, c_{i,k'}\} = \delta_{kk'}$, but there is an overlap matrix connecting both sets, $\{c^\dagger_{0,k}, c_{1,l}\} =_0 \langle k|l\rangle_1 = \mathcal{R}_{kl}$. For simplicity, I consider in the following $N_0 = N_1 = N$, but note that the most general case can be easily accommodated in the formalism. I also introduce the complement of the two bases $\bar{\mathcal{B}}_0 = \{c^\dagger_{0,k}, k = N + 1, \dots, \infty\}$ and $\bar{\mathcal{B}}_1 = \{c^\dagger_{1,k}, k = N + 1, \dots, \infty\}$ 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 transformation matrix $R$ (not to be confused with $\mathcal{R}$). I am assuming separable Hilbert spaces for which countable orthonormal bases exist, and therefore, the introduction of a (infinite dimensional) matrix $R$ makes sense. Let us also introduce the quasiparticle annihilation operators $\alpha_{i\mu}$ $(i = 0, 1)$, which annihilate $|\phi_i\rangle$ and are written in terms of the complete bases $\{c^\dagger_{i,k}\}^\infty$ through the standard definition

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

By using the following block structure for the Bogoliubov amplitudes $U_i$ and $V_i$,

$$V_i = \begin{pmatrix} \bar{V}_i & 0 \\ 0 & 0 \end{pmatrix}, \quad U_i = \begin{pmatrix} \bar{U}_i & 0 \\ 0 & d_i \end{pmatrix}, \tag{2}$$

where $\bar{V}_i$ and $\bar{U}_i$ are $N \times N$ matrices, one can accommodate into the formalism the set of $N$ quasiparticle operators $\alpha_{i\mu}$, with $\mu = 1, \dots, N$, corresponding to the quasiparticle operators expanded in the truncated bases $\mathcal{B}_i$. The $d_i$ are arbitrary unitary matrices that should not appear explicitly in the final expressions. It is also convenient to express the unitary matrix $R$ connecting $\mathcal{B}_0 \cup \bar{\mathcal{B}}_0$ and $\mathcal{B}_1 \cup \bar{\mathcal{B}}_1$ 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:

$$\hat{\mathcal{T}}_{01} c^\dagger_{0,k} \hat{\mathcal{T}}^\dagger_{01} = c^\dagger_{1,k}.$$

The $\hat{\mathcal{T}}_{01}$ operator can be a symmetry operator like a spatial translation, a rotation, or the dilatation operator when dealing with HO bases differing in their oscillator lengths. In all the cases (and this is an implicit requirement of the present development) the operator is the exponential of a one-body operator. Finally, let us introduce the HFB state $|\tilde{\phi}_1\rangle$ and the associated annihilation operators $\tilde{\alpha}_{1,\mu}$ defined by the relations

$$\hat{\mathcal{T}}_{01}|\tilde{\phi}_1\rangle = |\phi_1\rangle$$

and

$$\hat{\mathcal{T}}_{01}\tilde{\alpha}_{1,\mu}\hat{\mathcal{T}}^\dagger_{01} = \alpha_{1,\mu}.$$

The annihilation operators $\tilde{\alpha}_{1,\mu}$ share the Bogoliubov amplitudes with $\alpha_{1,\mu}$ but are expressed in the basis $\mathcal{B}_0$ instead:

$$\tilde{\alpha}_{1\mu} = \sum_{k=1}^{N} (\bar{U}_1^*)_{k\mu} c_{0,k} + (\bar{V}_1^*)_{k\mu} c^\dagger_{0,k}.$$

Let us also introduce the $\hat{\mathcal{T}}_B$ operator of the Bogoliubov transformation from $\alpha_{0,\mu}$ to $\tilde{\alpha}_{1,\mu}$:

$$\hat{\mathcal{T}}_B \alpha_{0,\mu} \hat{\mathcal{T}}_B^+ = \tilde{\alpha}_{1,\mu}$$

and

$$\hat{\mathcal{T}}_B|\phi_0\rangle = |\tilde{\phi}_1\rangle.$$

To compute the overlap of Eq. (1) it will prove convenient to write the operator $\hat{O}$ in terms of both bases $\{c^\dagger_{0,k}\}^\infty$ and $\{c^\dagger_{1,k}\}^\infty$ in a convenient way. For instance, for a two-body operator one uses

$$\hat{\upsilon} = \frac{1}{4}\sum_{k_1k_2l_1l_2} \tilde{\upsilon}^{01}_{k_1k_2l_1l_2} c^\dagger_{0k_1} c^\dagger_{0,k_2} c_{1,l_2} c_{1,l_1}, \tag{3}$$

where the antisymmetrized two-body matrix element is given by $\tilde{\upsilon}^{01}_{k_1k_2l_1l_2} = \upsilon^{01}_{k_1k_2l_1l_2} - \upsilon^{01}_{k_1k_2l_2l_1}$, with

$$\upsilon^{01}_{k_1k_2l_2l_1} =_0 \langle k_1k_2|\hat{\upsilon}|l_1l_2\rangle_1 \tag{4}$$

being the interaction's overlap matrix elements. The sums in Eq. (3) extend over the complete bases $\{c^\dagger_{0,k}\}^\infty$ and $\{c^\dagger_{1,k}\}^\infty$ to faithfully represent the operators. The advantage of Eq. (3) is that the annihilation operators acting on $|\phi_1\rangle$ lead to a linear combination of multi-quasiparticle excitations in which are all of them expressed in terms of basis $\mathcal{B}_1$ alone, whereas the creation operators' action to the left on $|\phi_0\rangle$ will do the same but in terms of $\mathcal{B}_0$. This is the key point to obtain expression for the overlaps depending solely in the bases used (and not their complements). The overlaps are computed by transforming to the quasiparticle representation and applying GWT. With the previous considerations one has to evaluate

$$\frac{\langle\phi_0|\alpha_{0,\mu_1}\dots\alpha_{0,\mu_M}\alpha^+_{1,\nu_M}\dots\alpha^+_{1,\nu_1}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \frac{\langle\phi_0|\alpha_{0,\mu_1}\dots\alpha_{0,\mu_M}\hat{\mathcal{T}}\alpha^+_{0,\nu_M}\dots\alpha^+_{0,\nu_1}|\phi_0\rangle}{\langle\phi_0|\hat{\mathcal{T}}|\phi_0\rangle}, \tag{5}$$

with $\hat{\mathcal{T}} = \hat{\mathcal{T}}_{01}\hat{\mathcal{T}}_B$ being the product of the exponential of one-body operators that can also be written as the exponential of a one-body operator [7]. To evaluate these overlaps I make heavy use of the results of Ref. [9] (denoted I hereafter). The main difference between the present results and those in I is that there I considered $\langle\phi_0|\hat{A}\hat{\mathcal{T}}|\phi_0\rangle/\langle\phi_0|\hat{\mathcal{T}}|\phi_0\rangle$, instead of having $\hat{\mathcal{T}}$ "in the middle" of $\hat{A}$ as is the case in the present formulation. Fortunately, one can use the decomposition given in Eq. (I.39) $\hat{\mathcal{T}} = \hat{\mathcal{T}}_1\hat{\mathcal{T}}_2\hat{\mathcal{T}}_3(\det R)^{1/2}$ (see also Ref. [7]), where each of the $\hat{\mathcal{T}}_i$ can be decomposed in turn as the product of three elementary transformations $\hat{\mathcal{T}}_i = \hat{\mathcal{T}}_i^{20}\hat{\mathcal{T}}_i^{11}\hat{\mathcal{T}}_i^{02}\mathcal{T}_i^{0}$, where $\mathcal{T}_i^{nm}$ represents the exponential of a one-body operator expressed as linear combinations of the product of $n$ quasiparticle creation ($\alpha_{0,\mu}^+$) and $m$ annihilation operators ($\alpha_{0,\mu}$) and $\mathcal{T}_i^0$ represents a constant factor. According to Eqs. (I.42)–(I.54) in I one has $\hat{\mathcal{T}}_1^{02} = \hat{\mathcal{T}}_3^{20} = \mathbb{I}$ and $\mathcal{T}_1^0 = \mathcal{T}_3^0 = 1$, which allows one to define the operators

$$\hat{\mathcal{T}}_L = \hat{\mathcal{T}}_1^{20}\hat{\mathcal{T}}_1^{11}\hat{\mathcal{T}}_2^{20}\hat{\mathcal{T}}_2^{11} \tag{6}$$

and

$$\hat{\mathcal{T}}_R = \hat{\mathcal{T}}_2^{02}\hat{\mathcal{T}}_3^{11}\hat{\mathcal{T}}_3^{02}, \tag{7}$$

such that $\hat{\mathcal{T}} = \hat{\mathcal{T}}_L\hat{\mathcal{T}}_R$ (up to an irrelevant $\mathcal{T}_2^0$ factor) and with the properties $\langle\phi_0|\hat{\mathcal{T}}_L = \langle\phi_0|$ and $\hat{\mathcal{T}}_R|\phi_0\rangle = |\phi_0\rangle$. One can use now the operators $\hat{\mathcal{T}}_L$ and $\hat{\mathcal{T}}_R$ to define the quasiparticle operators (satisfying CARs) $d_0$, $\bar{d}_0$, $b_0$, and $\bar{b}_0$ by means of the following relations:

$$\begin{pmatrix} d_0 \\ \bar{d}_0 \end{pmatrix} = \hat{\mathcal{T}}_L^{-1}\begin{pmatrix} \alpha_0 \\ \alpha_0^+ \end{pmatrix}\hat{\mathcal{T}}_L, \tag{8}$$

$$\begin{pmatrix} b_0 \\ \bar{b}_0 \end{pmatrix} = \hat{\mathcal{T}}_R\begin{pmatrix} \alpha_0 \\ \alpha_0^+ \end{pmatrix}\hat{\mathcal{T}}_R^{-1}, \tag{9}$$

and one can finally express the matrix element of Eq. (5) as the mean value

$$\langle\phi_0|d_{0,\mu_1}\dots d_{0,\mu_M}\bar{b}_{0,\nu_M}\dots\bar{b}_{0,\nu_1}|\phi_0\rangle, \tag{10}$$

where $d_0$ and $b_0$ are quasiparticle operators' linear combinations of $\alpha_0$ and $\alpha_0^+$. Therefore, one can use the standard Wick's theorem to evaluate Eq. (10) in terms of the contractions $\langle\phi_0|d_{0,\mu}\bar{b}_{0,\nu}|\phi_0\rangle$, $\langle\phi_0|d_{0,\mu}d_{0,\nu}|\phi_0\rangle$, and $\langle\phi_0|\bar{b}_{0,\mu}\bar{b}_{0,\nu}|\phi_0\rangle$. In order to obtain the expressions of the contractions one needs the explicit form of the $d_0$ and $\bar{b}_0$ operators in terms of $\alpha_0$ and $\alpha_0^+$. Using Eqs. (I.32), (I.A5), and (I.A6), one gets (using the notation of I)

$$\begin{pmatrix} d_0 \\ \bar{d}_0 \end{pmatrix} = \begin{pmatrix} D_{11} & D_{12} \\ 0 & D_{22} \end{pmatrix}\begin{pmatrix} \alpha_0 \\ \alpha_0^+ \end{pmatrix},$$

with

$$\begin{pmatrix} D_{11} & D_{12} \\ 0 & D_{22} \end{pmatrix} = \begin{pmatrix} T_{11}^{(1)} & T_{12}^{(1)} \\ 0 & T_{22}^{(1)} \end{pmatrix}\begin{pmatrix} \mathbb{I} & K^{(1)} \\ 0 & \mathbb{I} \end{pmatrix} \times \begin{pmatrix} e^{L^{(2)}} & 0 \\ 0 & e^{-(L^{(2)})^T} \end{pmatrix}.$$

In the same way and using Eqs. (I.35), (I.A7), and (I.51)–(I.54), one obtains

$$\begin{pmatrix} b_0 \\ \bar{b}_0 \end{pmatrix} = \begin{pmatrix} B_{11} & 0 \\ B_{21} & B_{22} \end{pmatrix}\begin{pmatrix} \alpha_0 \\ \alpha_0^+ \end{pmatrix},$$

with

$$\begin{pmatrix} B_{11} & 0 \\ B_{21} & B_{22} \end{pmatrix} = \begin{pmatrix} \mathbb{I} & 0 \\ -M^{(3)} & \mathbb{I} \end{pmatrix}\begin{pmatrix} e^{-L^{(3)}} & 0 \\ 0 & (e^{L^{(3)}})^T \end{pmatrix} \times \begin{pmatrix} \mathbb{I} & 0 \\ -M^{(2)} & \mathbb{I} \end{pmatrix}.$$

The relevant contractions are easily obtained:

$$\langle\phi_0|d_{0,\mu}\bar{b}_{0,\nu}|\phi_0\rangle \equiv C_{\mu\nu} = \left(D_{11}B_{22}^T\right)_{\mu\nu}, \tag{11}$$

$$\langle\phi_0|d_{0,\mu}d_{0,\nu}|\phi_0\rangle \equiv D_{\mu\nu} = \left(D_{11}D_{12}^T\right)_{\mu\nu}, \tag{12}$$

$$\langle\phi_0|\bar{b}_{0,\mu}\bar{b}_{0,\nu}|\phi_0\rangle \equiv E_{\mu\nu} = \left(B_{21}B_{22}^T\right)_{\mu\nu}. \tag{13}$$

Using the explicit form of the matrices $T_{ij}^{(1)}$, $M^{(2)}$, $M^{(3)}$, $L^{(2)}$, and $L^{(3)}$ given in I and their block decomposition in terms of the original basis and its complement, one obtains the desired expressions for the contractions. Using Eqs. (I.32a), (I.47), and (I.52), one arrives at

$$\frac{\langle\phi_0|\alpha_{0,\mu}\alpha_{1,\nu}^+|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \langle\phi_0|d_{0,\mu}\bar{b}_{0,\nu}|\phi_0\rangle = \begin{pmatrix} (A^T)^{-1} & \bullet \\ \bullet & \bullet \end{pmatrix}_{\mu\nu}.$$

Using Eqs. (I.32a), (I.46), and (I.32b), one obtains

$$\frac{\langle\phi_0|\alpha_{0,\mu}\alpha_{0,\nu}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle}\langle\phi_0|d_{0,\mu}d_{0,\nu}|\phi_0\rangle = \begin{pmatrix} -BA^{-1} & \bullet \\ \bullet & \bullet \end{pmatrix}_{\mu\nu}.$$

Finally, using Eqs. (I.48), (I.52), and (I.53), one gets

$$\frac{\langle\phi_0|\alpha_{1,\mu}^+\alpha_{1,\nu}^+|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \langle\phi_0|\bar{b}_{0,\mu}\bar{b}_{0,\nu}|\phi_0\rangle = \begin{pmatrix} -A^{-1}\bar{B} & \bullet \\ \bullet & \bullet \end{pmatrix}_{\mu\nu},$$

where the indices of the matrices $A$, $B$, and $\bar{B}$ (to be defined below) run over the original space spanned by the original bases and the symbol "$\bullet$" represents irrelevant matrices defined in the complementary subspaces. The matrices $A$, $B$, and $\bar{B}$ are defined through the relation

$$\begin{pmatrix} \bar{A} & B \\ \bar{B} & A \end{pmatrix} = \begin{pmatrix} \bar{U}_0^\dagger & \bar{V}_0^\dagger \\ \bar{V}_0^T & \bar{U}_0^T \end{pmatrix}\begin{pmatrix} \mathcal{R} & 0 \\ 0 & (\mathcal{R}^T)^{-1} \end{pmatrix}\begin{pmatrix} \bar{U}_1 & \bar{V}_1^* \\ \bar{V}_1 & \bar{U}_1^* \end{pmatrix}. \tag{14}$$

With the above results it is evident that the evaluation of the overlap $\langle\phi_0|c_{0k_1}^\dagger c_{0,k_2}^\dagger c_{1,l_2}c_{1,l_1}|\phi_1\rangle/\langle\phi_0|\phi_1\rangle$ can be carried out according to the rules of the GWT in terms of the contractions

$$\rho_{lk}^{01} = \frac{\langle\phi_0|c_{0,k}^\dagger c_{1,l}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \left(V_1^*C^TV_0^T\right)_{lk} = \begin{pmatrix} \bar{V}_1^*(A)^{-1}\bar{V}_0^T & 0 \\ 0 & 0 \end{pmatrix} \tag{15}$$

$$\bar{\kappa}_{k_1k_2}^{01} = \frac{\langle\phi_0|c_{0,k_1}^\dagger c_{0,k_2}^\dagger|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \left(V_0U_0^+ + V_0DV_0^T\right)_{k_1k_2} = \begin{pmatrix} \bar{V}_0\bar{U}_0^+ - \bar{V}_0BA^{-1}\bar{V}_0^T & 0 \\ 0 & 0 \end{pmatrix} \tag{16}$$

$$\kappa_{l_1l_2}^{10} = \frac{\langle\phi_0|c_{1,l_1}c_{1,l_2}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = (U_1V_1^+ + V_1^*EV_1^+)_{l_1l_2} = \begin{pmatrix} \bar{U}_1\bar{V}_1^+ - \bar{V}_1^*A^{-1}\bar{B}\bar{V}_1^+ & 0 \\ 0 & 0 \end{pmatrix}. \tag{17}$$

The result shows that the contractions are different from 0 only when the single-particle indexes $l$ and $k$ belong to the subspace spanned by bases $\mathcal{B}_0$ and $\mathcal{B}_1$, and therefore, the complementary subspace (of infinite dimension) is not required. Finally, taking into account the unitarity [3] of the matrices

$$\bar{W}_i = \begin{pmatrix} \bar{U}_i & \bar{V}_i^* \\ \bar{V}_i & \bar{U}_i^* \end{pmatrix},$$

it is possible to derive from Eq. (14) a set of identities like $\bar{V}_0 B + \bar{U}_0^* A = (\mathcal{R}_1^T)^{-1}\bar{U}_1^*$ that are essential to arrive at the final result for the contractions

$$\rho^{01}_{lk} = \left[\bar{V}_1^* A^{-1} \bar{V}_0^T\right]_{lk}, \tag{18}$$

$$\bar{\kappa}^{01}_{k_1k_2} = -\left[\left(\mathcal{R}^T\right)^{-1} \bar{U}_1^* A^{-1} \bar{V}_0^T\right]_{k_1k_2}, \tag{19}$$

$$\kappa^{10}_{l_1l_2} = \left[\bar{V}_1^* A^{-1} \bar{U}_0^T (\mathcal{R}^T)^{-1}\right]_{l_1l_2}, \tag{20}$$

if the indexes belong to the subspace spanned by bases $\mathcal{B}_0$ and $\mathcal{B}_1$ and 0 otherwise. The matrix $A$, playing a central role in the above expressions, can be obtained from Eq. (14) and is given by

$$A = \bar{U}_0^T (\mathcal{R}^T)^{-1} \bar{U}_1^* + \bar{V}_0^T \mathcal{R} \bar{V}_1^*. \tag{21}$$

For instance, the overlap of a one-body operator $\hat{O} = \sum_{ij} O^{01}_{kl} c^\dagger_{0,k} c_{1,l}$, with $O^{01}_{kl} = {}_0\langle k|\hat{O}|l\rangle_1$, is given by $\mathrm{Tr}(O^{01}\rho^{01})$ in agreement with Eq. (I.82). Please note that with the present formalism the formal developments of Sec V of I leading from Eq. (I.75) to Eq. (I.82) are not required. The new formulation presented in this paper does not affect the expression for the overlap that is still given by Eq. (I.58):

$$\langle\phi_0|\phi_1\rangle = \sqrt{\det A \det \mathcal{R}}. \tag{22}$$

This expression suffers from the sign indetermination of the square root already present in the formula of Onishi and Yoshida [6]. This indetermination can be resolved by using the Pfaffian formula for the overlap derived in Ref. [10]. The formula obtained there was further generalized in Ref. [11] to deal with the situation discussed here [see Eqs. (59)– (61) of that reference]. Later on, another, less general, Pfaffian formula for the overlap was given in Ref. [24].

In the present derivation, I have assumed that both bases $\mathcal{B}_0$ and $\mathcal{B}_1$ have the same dimensionality and the overlap matrix $\mathcal{R}$ is a square, invertible one. If this is not the case and, for instance, base $\mathcal{B}_0$ has a dimension $N_0$ smaller than $N_1$ (the dimension of $\mathcal{B}_1$), one can complete $\mathcal{B}_0$ with $N_1 - N_0$ orthogonal vectors and assign occupancy 0 to them in the spirit of Eq. (2) in order to get a square overlap matrix.

The formulas can be further simplified by introducing the LU decomposition of the overlap matrix $\mathcal{R}$,

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

where $L_0$ and $L_1$ are lower triangular matrices. It introduces 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 following definitions,

$$\tilde{U}_0 = (L_0^*)^{-1} \bar{U}_0 L_0^+, \quad \tilde{V}_0 = L_0^+ \bar{V}_0 L_0^+, \tag{23}$$

$$\tilde{U}_1 = (L_1^*)^{-1} \bar{U}_1 L_1^+, \quad \tilde{V}_1 = L_1^+ \bar{V}_1 L_1^+, \tag{24}$$

which allow one to obtain quantities not depending explicitly on $\mathcal{R}$ like

$$\tilde{A} = \tilde{U}_0^T \tilde{U}_1^* + \tilde{V}_0^T \tilde{V}_1^* = L_0^* A L_1^T. \tag{25}$$

The overlap is now written as

$$\langle\phi_0|\phi_1\rangle = \sqrt{\det \tilde{A}}. \tag{26}$$

It is also convenient to introduce the contractions

$$\tilde{\rho}^{01}_{lk} = \left[\tilde{V}_1^* \tilde{A}^{-1} \tilde{V}_0^T\right]_{lk} = L_1^T \rho^{01} L_0^*, \tag{27}$$

$$\tilde{\bar{\kappa}}^{01}_{k_1k_2} = -\left[\tilde{U}_1^* \tilde{A}^{-1} \tilde{V}_0^T\right]_{k_1k_2} = L_0^+ \bar{\kappa}^{01} L_0^*, \tag{28}$$

$$\tilde{\kappa}^{10}_{l_1l_2} = \left[\tilde{V}_1^* \tilde{A}^{-1} \tilde{U}_0^T\right]_{l_1l_2} = L_1^T \kappa^{01} L_1. \tag{29}$$

Using them and the matrix elements $\tilde{O} = (L_0^*)^{-1} O^{01} (L_1^T)^{-1}$,[1] one gets $\mathrm{Tr}(\tilde{O}\tilde{\rho}^{01})$ for the overlap of a one-body operator. Similar considerations apply to the overlap of two-body operators. Introducing the two-body matrix element in the biorthogonal basis $\upsilon^B_{ijkl} = {}_0(ij|\hat{\upsilon}|kl)_1$ and related to $\upsilon^{01}_{ijkl}$ by

$$\upsilon^B = (L_0^*)^{-1} (L_0^*)^{-1} \upsilon^{01} \left(L_1^T\right)^{-1} \left(L_1^T\right)^{-1},$$

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

$$\frac{\langle\phi_0|\hat{\upsilon}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \frac{1}{2}\mathrm{Tr}\left[\tilde{\Gamma}^{01}\tilde{\rho}^{01}\right] - \frac{1}{2}\mathrm{Tr}\left[\tilde{\Delta}^{01}\tilde{\bar{\kappa}}^{01}\right], \tag{30}$$

which is again the standard expression but defined in terms of Eqs. (27), (28), and (29) and the definitions above. The advantage of the definitions in Eqs. (25), (27), (28), and (29) is that they have exactly the same expression as the formulas available in the literature for complete basis but expressed in terms of the "tilde" $U$ and $V$ matrices of Eqs. (23) and (24). 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 $\mathcal{R}$. Let us finish by writing down the expression of the density in coordinate space representation,

$$\rho^{01}(\vec{r}) = \frac{\langle\phi_0|\hat{\rho}|\phi_1\rangle}{\langle\phi_0|\phi_1\rangle} = \sum_{ij} \varphi^*_{0i}(\vec{r})\varphi_{1j}(\vec{r})\rho^{01}_{ji},$$

often used along with zero-range interactions.

Before finishing the presentation there are a few comments worth mentioning.

(i) The simple form of the contractions of Eqs. (18), (19), and (20) and the fact that they are only different from 0 when the indexes belong to the subspace spanned by bases $\mathcal{B}_0$ and $\mathcal{B}_1$ is a direct consequence of the definitions of Eqs. (15), (16), and (17) mixing single-particle operators of both bases. Those definitions are useful because the operators are expressed in the mixed form of Eq. (3).

(ii) The use of operators mixing creation and annihilation operators of both bases as in Eq. (3) and the expressions of Eqs. (15), (16), and (17) were already given in Ref. [22] without proof and without a justification

[1] The matrix elements $\tilde{O}_{lk}$ are the ones of the operator $\hat{O}$ in the biorthogonal bases ${}_0(l|$ and $|k)_1$, i.e., $\tilde{O}_{lk} = {}_0(l|\hat{O}|k)_1 = \sum (L_0^*)^{-1}_{li} {}_0\langle i|\hat{O}|j\rangle_1 (L_1^T)^{-1}_{jk}$.

of their interpretation as the contractions appearing in the GWT.

In this paper I have presented a modified version of the developments of Ref. [9] that simplifies the application of the generalized Wick's theorem for the calculation of operator overlaps in the case of using two different nonequivalent bases for the two HFB states entering the overlap. Applications of this formalism to the case of harmonic oscillator bases with different oscillator lengths will be discussed in a future publication.

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