Appendix A
Hartree-Fock-Bogoliubov Algorithm

The HFB formalism described in Chap. 1 is central to the work presented in this manuscript. In this section, we present an algorithm that implements this formalism and that was used to obtain the results discussed throughout the manuscript. This algorithm was discussed in a previous publication [4], and is repeated here for completeness and for the reader's convenience. Other examples of Hartree-Fock and Hartree-Fock-Bogoliubov algorithms and codes can be readily found in the literature [1–3].

The main steps are shown in Algorithm 1. A list of basis states is generated in Step 1 using the formalism described in Sect. 2.2, and grouped according to symmetries required by the user. These groups define the block structure of the various field matrices in the computation. If a starting solution is available, the corresponding densities (ρ_n, ρ_p) and pairing tensors (κ_n, κ_p) are read in along with any Lagrange multipliers for the constraints in Step 3. At this point, the main HFB loop begins. Various field matrices are calculated in Step 5 for the kinetic energy operator (T_n, T_p), the mean field (Γ_n, Γ_p), and the pairing field (Δ_n, Δ_p) as described in Chaps. 1 and 2. These fields are assembled into the HFB matrix in Eq. (1.13), and diagonalized in Step 6 to obtain the U and V matrices. From these new U and V matrices, new densities and pairing tensors for the neutrons and protons in Step 7. Next, the change in generalized density from the previous iteration $(i-1)$ is calculated in Step 8 to gauge the convergence of the solution: $\varepsilon = \sup|R(i) - R(i-1)|$. A mixing parameter α between iterations is calculated based on the value of ε in Step 9 according to the formula [4]

$$\alpha = \begin{cases} \alpha_{\max} & \varepsilon \geq \varepsilon_{\max} \\ \alpha_{\max}\frac{\varepsilon-\varepsilon_{\min}}{\varepsilon_{\max}-\varepsilon_{\min}} & \varepsilon_{\min} < \varepsilon \leq \varepsilon_{\max} \\ 0 & \varepsilon < \varepsilon_{\min} \end{cases} \tag{A.1}$$

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with typical values $\varepsilon_{\text{min}} = 10^{-4}$, $\varepsilon_{\text{max}} = 10^{-1}$, and $\alpha_{\text{max}} = 0.8$. The solutions are then mixed in Step 10,

$$R(i) \leftarrow (1-\alpha)R(i) + \alpha R(i-1) \tag{A.2}$$

The Lagrange multipliers and generalized density are adjusted in Steps 11 and 12, respectively, as described in Sect. 1.5.2 to satisfy any constraints imposed by the user. The HFB loop terminates if $\varepsilon < \varepsilon_{\text{min}}$ for a set number of consecutive iterations (typically 3) to ensure that the solution is stable.

Algorithm 1 HFB algorithm pseudocode

```
1:  Generate basis state quantum numbers (n_r, Λ, n_z, σ)
2:  Subdivide basis into blocks, according to imposed symmetries
3:  Read initial generalized density R and Lagrange multipliers λ_i
4:  repeat
5:      Construct Hamiltonian fields
6:      Diagonalize the HFB Hamiltonian (separately for neutrons and protons)
7:      Construct the new generalized density
8:      Calculate maximum change in generalized density
9:      Adjust mixing parameter
10:     Mix generalized density from this iteration with the one from the previous iteration
11:     Adjust Lagrange multipliers
12:     Adjust generalized density
13: until ϵ small enough
```

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Appendix B
Exact Solution of the Multi-O (4) Model

The exact solution for this model (introduced in [2–5] and summarized in Sect. 1.6.1) is obtained by using quasispin methods (see, e.g., chapter 7 in [1]). For this, we first introduce an additional operator

$$\hat{B}^\dagger = \sum_j \hat{B}_j^\dagger$$
$$\hat{B}_j^\dagger = \sum_{m>0} \sigma_{jm} a_{jm}^\dagger a_{j\bar{m}}^\dagger$$

and then define the quasispin operators [2–4][1]

$$\begin{aligned} \hat{K}_j^+ &\equiv \frac{1}{2}\left(\hat{A}_j^\dagger + \hat{B}_j^\dagger\right) \\ \hat{K}_j^- &\equiv \frac{1}{2}\left(\hat{A}_j + \hat{B}_j\right) \\ \hat{K}_j^0 &\equiv \frac{1}{4}\left(\hat{N}_j + \hat{D}_j - \Omega_j\right) \end{aligned} \tag{B.1}$$

and

$$\begin{aligned} \hat{L}_j^+ &\equiv \frac{1}{2}\left(\hat{A}_j^\dagger - \hat{B}_j^\dagger\right) \\ \hat{L}_j^- &\equiv \frac{1}{2}\left(\hat{A}_j - \hat{B}_j\right) \\ \hat{L}_j^0 &\equiv \frac{1}{4}\left(\hat{N}_j - \hat{D}_j - \Omega_j\right) \end{aligned} \tag{B.2}$$

[1] Note the factor 1/4 in the definitions of $\hat{K}_j^0$ and $\hat{L}_j^0$ which is consistent with the definitions in [2], but not [3, 4].

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The sets $\left\{\hat{K}_j^+, \hat{K}_j^-, \hat{K}_j^0\right\}$ and $\left\{\hat{L}_{j,}^+, \hat{L}_j^-, \hat{L}_j^0\right\}$ separately form SU (2) algebras, and any two elements of different sets commute [3]. In particular, it can be readily verified that

$$\begin{aligned}
\left[\hat{K}_j^+, \hat{K}_j^-\right] &= 2\hat{K}_j^0 \\
\left[\hat{K}_j^0, \hat{K}_j^\pm\right] &= \pm\hat{K}_j^\pm \\
\left[\hat{K}_j^-, \hat{L}_j^+\right] &= 0 \\
\left[\hat{L}_j^+, \hat{L}_j^-\right] &= 2\hat{L}_j^0 \\
\left[\hat{L}_j^0, \hat{L}_j^\pm\right] &= \pm\hat{L}_j^\pm
\end{aligned} \tag{B.3}$$

with all other commutators (e.g., between operators in j and j' where $j \neq j'$) equal to zero. We can then write

$$\begin{aligned}
\hat{A}_j^\dagger &= \hat{K}_j^+ + \hat{L}_j^+ \\
\hat{A}_j &= \hat{K}_j^- + \hat{L}_j^- \\
\hat{D}_j &= 2\left(\hat{K}_j^0 - \hat{L}_j^0\right) \\
\hat{N}_j &= 2\left(\hat{K}_j^0 + \hat{L}_j^0\right) + \Omega_j
\end{aligned} \tag{B.4}$$

so that the components in Eq. (1.79) become

$$\hat{H}_0 = \sum_j e_j^0 \left[2\left(\hat{K}_j^0 + \hat{L}_j^0\right) + \Omega_j\right] \tag{B.5}$$

$$\hat{H}_Q = 2\chi \sum_{j,j'} d_j d_{j'} \left(\hat{K}_j^0 - \hat{L}_j^0\right)\left(\hat{K}_{j'}^0 - \hat{L}_{j'}^0\right) \tag{B.6}$$

$$\hat{H}_P = -\frac{1}{2}G \sum_{j,j'} \left[\left(\hat{K}_j^+ + \hat{L}_j^+\right)\left(\hat{K}_{j'}^- + \hat{L}_{j'}^-\right) + \left(\hat{K}_{j'}^- + \hat{L}_{j'}^-\right)\left(\hat{K}_j^+ + \hat{L}_j^+\right)\right] \tag{B.7}$$

B.1 Useful Results for the Quasi-spin Algebra

B.1.1 The Action of $\hat{K}_j^0$ on the State $\left(\hat{K}_j^+\right)^n |0\rangle$

Let us first calculate the effect of $\hat{K}_j^0$ on the particle vacuum $|0\rangle$ where we recall that (see Eq. (B.1))

$$\hat{K}_j^0 \equiv \frac{1}{4}\left(\hat{N}_j + \hat{D}_j - \Omega_j\right)$$

and therefore, using the definitions of the operators $\hat{N}_j$ and $\hat{D}_j$ in Eqs. (1.81) and (1.83), respectively, we find

$$\hat{K}_j^0 |0\rangle = -\frac{\Omega_j}{4} |0\rangle \tag{B.8}$$

Next, we wish to calculate $\hat{K}_j^0 \left(\hat{K}_j^+\right)^n |0\rangle$ for a given integer n with $0 \leq n \leq \Omega_j/2$. Using the $SU(2)$ commutators in Eq. (B.3) we write for example

$$\begin{aligned}\hat{K}_j^0 \hat{K}_j^+ &= \left[\hat{K}_j^0, \hat{K}_j^+\right] + \hat{K}_j^+ \hat{K}_j^0 \\ &= \hat{K}_j^+ \left(1 + \hat{K}_j^0\right)\end{aligned}$$

More generally, if for a given integer k we have

$$\hat{K}_j^0 \left(\hat{K}_j^+\right)^k = \left(\hat{K}_j^+\right)^k \left[k + \hat{K}_j^0\right]$$

then we can show that

$$\begin{aligned}\hat{K}_j^0 \left(\hat{K}_j^+\right)^{k+1} &= \hat{K}_j^0 \left(\hat{K}_j^+\right)^k \hat{K}_j^+ \\ &= \left(\hat{K}_j^+\right)^k \left[k + \hat{K}_j^0\right] \hat{K}_j^+ \\ &= k\left(\hat{K}_j^+\right)^{k+1} + \left(\hat{K}_j^+\right)^k \left[\hat{K}_j^+ \left(1 + \hat{K}_j^0\right)\right] \\ &= \left(\hat{K}_j^+\right)^{k+1} \left[k + 1 + \hat{K}_j^0\right]\end{aligned}$$

Therefore, by induction, we conclude that for any integer $n \geq 0$,

$$\hat{K}_j^0 \left(\hat{K}_j^+\right)^n = \left(\hat{K}_j^+\right)^n \left(n + \hat{K}_j^0\right) \tag{B.9}$$

and we can use this with Eq. (B.8) to calculate Eq. (A.8a) in [4]

$$\boxed{\hat{K}_j^0 \left(\hat{K}_j^+\right)^n |0\rangle = \left(n - \frac{\Omega_j}{4}\right) \left(\hat{K}_j^+\right)^n |0\rangle} \tag{B.10}$$

with a similar equation for the $\hat{L}_j^0$ and $\hat{L}_j^+$ operators defined in Eq. (B.2),

$$\boxed{\hat{L}_j^0 \left(\hat{L}_j^+\right)^n |0\rangle = \left(n - \frac{\Omega_j}{4}\right) \left(\hat{L}_j^+\right)^n |0\rangle} \tag{B.11}$$

B.1.2 The Action of $\hat{K}_j^-$ on the State $\left(\hat{K}_j^+\right)^n |0\rangle$

Using the $SU(2)$ algebra commutators in Eq. (B.3) we write

$$\begin{aligned}
\hat{K}_j^- \hat{K}_j^+ &= \left[\hat{K}_j^-, \hat{K}_j^+\right] + \hat{K}_j^+ \hat{K}_j^- \\
&= -2\hat{K}_j^0 + \hat{K}_j^+ \hat{K}_j^-
\end{aligned}$$

We use this result to calculate for any integer $n > 0$

$$\hat{K}_j^- \left(\hat{K}_j^+\right)^n = \left(-2\hat{K}_j^0 + \hat{K}_j^+ \hat{K}_j^-\right) \left(\hat{K}_j^+\right)^{n-1}$$

and with the help of Eq. (B.9) this gives a recurrence relation

$$\hat{K}_j^- \left(\hat{K}_j^+\right)^n = -2\left(\hat{K}_j^+\right)^{n-1} \left(n - 1 + \hat{K}_j^0\right) + \hat{K}_j^+ \left[\hat{K}_j^- \left(\hat{K}_j^+\right)^{n-1}\right] \tag{B.12}$$

If we apply this recurrence relation repeatedly to the right-hand side we find

$$\begin{aligned}
\hat{K}_j^- \left(\hat{K}_j^+\right)^n &= -2\left(\hat{K}_j^+\right)^{n-1} \left[(n-1) + (n-2) + \ldots + 1 + n\hat{K}_j^0\right] \\
&\quad + \left(\hat{K}_j^+\right)^n \hat{K}_j^- \\
&= -2\left(\hat{K}_j^+\right)^{n-1} \left[\frac{1}{2} n(n-1) + n\hat{K}_j^0\right] + \left(\hat{K}_j^+\right)^n \hat{K}_j^- \\
&= \left(\hat{K}_j^+\right)^{n-1} \left[n(1-n) - 2n\hat{K}_j^0\right] + \left(\hat{K}_j^+\right)^n \hat{K}_j^-
\end{aligned} \tag{B.13}$$

Using Eqs. (B.8) and (B.13), and the (easily verified) fact that $\hat{K}_j^- |0\rangle = 0$, we now calculate

$$\boxed{\hat{K}_j^- \left(\hat{K}_j^+\right)^n |0\rangle = n\left(\frac{\Omega_j}{2} - n + 1\right)\left(\hat{K}_j^+\right)^{n-1} |0\rangle} \tag{B.14}$$

We can derive a similar relation for the $\hat{L}_j^-$ and $\hat{L}_j^+$ operators defined in Eq. (B.2),

$$\boxed{\hat{L}_j^- \left(\hat{L}_j^+\right)^n |0\rangle = n\left(\frac{\Omega_j}{2} - n + 1\right)\left(\hat{L}_j^+\right)^{n-1} |0\rangle} \tag{B.15}$$

B.1.3 Normalization of the State $\left(\hat{K}_j^+\right)^n |0\rangle$

We define the state

$$|n\rangle \equiv C_n \left(\hat{K}_j^+\right)^n |0\rangle$$

where C_n is a normalization constant that we wish to determine such that

$$\langle n|\,n\rangle = |C_n|^2 \left\langle 0 \middle| \left(\hat{K}_j^-\right)^n \left(\hat{K}_j^+\right)^n \middle| 0 \right\rangle = 1$$

Now we use Eq. (B.14) to write

$$\begin{aligned}\left\langle 0 \middle| \left(\hat{K}_j^-\right)^n \left(\hat{K}_j^+\right)^n \middle| 0 \right\rangle &= \left\langle 0 \middle| \left(\hat{K}_j^-\right)^{n-1} \hat{K}_j^- \left(\hat{K}_j^+\right)^n \middle| 0 \right\rangle \\ &= n\left(\frac{\Omega_j}{2} - n + 1\right)\left\langle 0 \middle| \left(\hat{K}_j^-\right)^{n-1} \left(\hat{K}_j^+\right)^{n-1} \middle| 0 \right\rangle\end{aligned}$$

and therefore, for any integer $n > 0$

$$\boxed{|C_n|^2 = \frac{|C_{n-1}|^2}{n\left(\frac{\Omega_j}{2} - n + 1\right)}} \tag{B.16}$$

with a similar normalization coefficient for the state $\left(\hat{L}_j^+\right)^n |0\rangle$. Note that Eq. (B.16) only gives a recurrence relation for the normalization coefficients, however that is all we will need in order to calculate the matrix elements of the multi-$O(4)$ Hamiltonian.

B.2 Many-Body Basis States

We introduce the basis states for the model [4]

$$|n_K, n_L\rangle = \prod_j \left|n_{K_j}, n_{L_j}\right\rangle \tag{B.17}$$

where the integers n_{K_j} and n_{L_j} satisfy the relations

$$0 \le n_{K_j}, n_{L_j} \le \frac{\Omega_j}{2}$$

and

$$\sum_j \left(n_{K_j} + n_{L_j}\right) = \frac{N}{2}$$

In each j shell, we define the states

$$\left|n_{K_j}, n_{L_j}\right\rangle = C_{n_{K_j}} C_{n_{L_j}} \left(\hat{K}_j^+\right)^{n_{K_j}} \left(\hat{L}_j^+\right)^{n_{L_j}} |0\rangle \tag{B.18}$$

where $|0\rangle$ is the particle vacuum, and $C_{n_{K_j}}$ and $C_{n_{L_j}}$ are normalization coefficients given by the recurrence relation in Eq. (B.16). We now calculate the effect of the quasispin operators on the basis states. Using Eqs. (B.10) and (B.11), we readily show that

$$\boxed{\hat{K}_j^0 \left|n_{K_j}, n_{L_j}\right\rangle = \left(n_{K_j} - \frac{\Omega_j}{4}\right) \left|n_{K_j}, n_{L_j}\right\rangle} \tag{B.19}$$

and

$$\boxed{\hat{L}_j^0 \left|n_{K_j}, n_{L_j}\right\rangle = \left(n_{L_j} - \frac{\Omega_j}{4}\right) \left|n_{K_j}, n_{L_j}\right\rangle} \tag{B.20}$$

Next, we calculate

$$\begin{aligned}
\hat{K}_j^+ \left|n_{K_j}, n_{L_j}\right\rangle &= \frac{C_{n_{K_j}}}{C_{n_{K_j}+1}} C_{n_{K_j}+1} C_{n_{L_j}} \left(\hat{K}_j^+\right)^{n_{K_j}+1} \left(\hat{L}_j^+\right)^{n_{L_j}} |0\rangle \\
&= \frac{C_{n_{K_j}}}{C_{n_{K_j}+1}} \left|n_{K_j}+1, n_{L_j}\right\rangle
\end{aligned}$$

and if we assume, without loss of generality, that the normalization coefficients are real and positive we can use Eq. (B.16) to write

$$\boxed{\hat{K}_j^+ \left|n_{K_j}, n_{L_j}\right\rangle = \sqrt{\left(n_{K_j}+1\right)\left(\frac{\Omega_j}{2} - n_{K_j}\right)} \left|n_{K_j}+1, n_{L_j}\right\rangle} \tag{B.21}$$

and similarly,

$$\boxed{\hat{L}_j^+ \left|n_{K_j}, n_{L_j}\right\rangle = \sqrt{\left(n_{L_j}+1\right)\left(\frac{\Omega_j}{2} - n_{L_j}\right)} \left|n_{K_j}, n_{L_j}+1\right\rangle} \tag{B.22}$$

Finally, we use Eq. (B.13) to write

$$\begin{aligned}
\hat{K}_j^- \left|n_{K_j}, n_{L_j}\right\rangle &= C_{n_{K_j}} C_{n_{L_j}} \left\{ \left(\hat{K}_j^+\right)^{n_{K_j}-1} \left[n_{K_j}\left(1-n_{K_j}\right) - 2n_{K_j}\hat{K}_j^0\right] \right. \\
&\quad \left. + \left(\hat{K}_j^+\right)^{n_{K_j}} \hat{K}_j^- \right\} \left(\hat{L}_j^+\right)^{n_{L_j}} |0\rangle \\
&= \left[n_{K_j}\left(1-n_{K_j}\right) - 2n_{K_j}\left(-\frac{\Omega_j}{4}\right)\right] \frac{C_{n_{K_j}}}{C_{n_{K_j}-1}} \left|n_{K_j}-1, n_{L_j}\right\rangle
\end{aligned}$$

Then we use Eq. (B.16), along with the assumption that the normalization coefficients are real and positive, to write

$$\boxed{\hat{K}_j^- \left|n_{K_j}, n_{L_j}\right\rangle = \sqrt{n_{K_j}\left(\frac{\Omega_j}{2} - n_{K_j}+1\right)} \left|n_{K_j}-1, n_{L_j}\right\rangle} \tag{B.23}$$

with a similar relation for the $\hat{L}_j^-$ operator,

$$\boxed{\hat{L}_j^- \left|n_{K_j}, n_{L_j}\right\rangle = \sqrt{n_{L_j}\left(\frac{\Omega_j}{2} - n_{L_j}+1\right)} \left|n_{K_j}, n_{L_j}-1\right\rangle} \tag{B.24}$$

These results are in agreement with those found in Appendix A of [4].

B.3 Matrix Elements of the Model Hamiltonian

With Eqs. (B.19), (B.20), (B.21), (B.22), (B.23), and (B.24) we have all the necessary elements to calculate the matrix elements of the Hamiltonian (with components given by Eqs. (B.5), (B.6), and (B.7) in the quasispin representation) between the basis states in Eq. (B.17). Using Eqs. (B.19) and (B.20) we can show that

$$\left[2\left(\hat{K}_j^0+\hat{L}_j^0\right)+\Omega_j\right]\left|n_{K_j},n_{L_j}\right\rangle = 2\left(n_{K_j}+n_{L_j}\right)\left|n_{K_j},n_{L_j}\right\rangle$$

from which we deduce

$$\boxed{\left\langle n_K,n_L\left|\hat{H}_0\right|n'_K,n'_L\right\rangle = 2\left(\prod_j \delta_{n_{K_j},n'_{K_j}}\delta_{n_{L_j},n'_{L_j}}\right)\sum_j e_j^0\left(n_{K_j}+n_{L_j}\right)} \tag{B.25}$$

Next, for the quadrupole interaction, Eq. (B.6), we can use Eqs. (B.19) and (B.20) again to show that

$$\begin{aligned}\left(K_i^0-L_i^0\right)\left(K_j^0-L_j^0\right)\left|n_{K_i},n_{L_i}\right\rangle\left|n_{K_j},n_{L_j}\right\rangle &= \left(n_{K_i}-n_{L_j}\right)\left(n_{K_j}-n_{L_j}\right)\\ &\quad\times\left|n_{K_i},n_{L_i}\right\rangle\left|n_{K_j},n_{L_j}\right\rangle\end{aligned}$$

from which we deduce

$$\boxed{\begin{aligned}\left\langle n_K,n_L\left|\hat{H}_Q\right|n'_K,n'_L\right\rangle &= -2\chi\left(\prod_j \delta_{n_{K_j},n'_{K_j}}\delta_{n_{L_j},n'_{L_j}}\right)\\ &\quad\times\sum_{i,j} d_i d_j\left(n_{K_i}-n_{L_j}\right)\left(n_{K_j}-n_{L_j}\right)\end{aligned}} \tag{B.26}$$

Finally, we calculate the matrix elements for the pairing term in the Hamiltonian in Eq. (B.7). To simplify the notation, we introduce the quantity

$$p_j(n) \equiv \sqrt{n\left(\frac{\Omega_j}{2}-n+1\right)}$$

for $0 \le n \le \Omega_j/2+1$. Then, with the help of Eqs. (B.21), (B.22), (B.23), and (B.24), we can show that

$$\begin{aligned}\left\langle n_{K_j},n_{L_j}\left|\left(\hat{K}_j^+ +\hat{L}_j^+\right)\right|n'_{K_j},n'_{L_j}\right\rangle &= p_j\left(n_{K_j}\right)\delta_{n_{K_j},n'_{K_j}+1}\delta_{n_{L_j},n'_{L_j}}\\ &\quad+p_j\left(n_{L_j}\right)\delta_{n_{K_j},n'_{K_j}}\delta_{n_{L_j},n'_{L_j}+1}\end{aligned}$$

and

$$\left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^- + \hat{L}_j^- \right) \right| n'_{K_j}, n'_{L_j} \right\rangle = p_j \left(n_{K_j} + 1 \right) \delta_{n_{K_j}, n'_{K_j} - 1} \delta_{n_{L_j}, n'_{L_j}} + p_j \left(n_{L_j} + 1 \right) \delta_{n_{K_j}, n'_{K_j}} \delta_{n_{L_j}, n'_{L_j} - 1}$$

and

$$\begin{aligned} &\left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^- + \hat{L}_j^- \right) \left(\hat{K}_j^+ + \hat{L}_j^+ \right) \right| n'_{K_j}, n'_{L_j} \right\rangle \\ &= \delta_{n_{K_j}, n'_{K_j}} \delta_{n_{L_j}, n'_{L_j}} \left[p_j^2 \left(n_{K_j} + 1 \right) + p_j^2 \left(n_{L_j} + 1 \right) \right] \\ &+ \delta_{n_{K_j}, n'_{K_j} + 1} \delta_{n_{L_j}, n'_{L_j} - 1} p_j \left(n_{K_j} \right) p_j \left(n_{L_j} + 1 \right) \\ &+ \delta_{n_{K_j}, n'_{K_j} - 1} \delta_{n_{L_j}, n'_{L_j} + 1} p_j \left(n_{K_j} + 1 \right) p_j \left(n_{L_j} \right) \end{aligned}$$

and

$$\begin{aligned} &\left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^+ + \hat{L}_j^+ \right) \left(\hat{K}_j^- + \hat{L}_j^- \right) \right| n'_{K_j}, n'_{L_j} \right\rangle \\ &= \delta_{n_{K_j}, n'_{K_j}} \delta_{n_{L_j}, n'_{L_j}} \left[p_j^2 \left(n_{K_j} \right) + p_j^2 \left(n_{L_j} \right) \right] \\ &+ \delta_{n_{K_j}, n'_{K_j} - 1} \delta_{n_{L_j}, n'_{L_j} + 1} p_j \left(n_{K_j} + 1 \right) p_j \left(n_{L_j} \right) \\ &+ \delta_{n_{K_j}, n'_{K_j} + 1} \delta_{n_{L_j}, n'_{L_j} - 1} p_j \left(n_{K_j} \right) p_j \left(n_{L_j} + 1 \right) \end{aligned}$$

We now combine these four results to calculate the full matrix element for the pairing term,

$$\boxed{\begin{aligned} &\left\langle n_K, n_L \left| \hat{H}_P \right| n'_K, n'_L \right\rangle \\ &\quad = -\tfrac{1}{2} G \textstyle\sum_j \left(\prod_{i \neq j} \delta_{n_{K_i}, n'_{K_i}} \delta_{n_{L_i}, n'_{L_i}} \right) \\ &\qquad \times \left\{ \left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^+ + \hat{L}_j^+ \right) \left(\hat{K}_j^- + \hat{L}_j^- \right) \right| n'_{K_j}, n'_{L_j} \right\rangle \right. \\ &\qquad \left. + \left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^- + \hat{L}_j^- \right) \left(\hat{K}_j^+ + \hat{L}_j^+ \right) \right| n'_{K_j}, n'_{L_j} \right\rangle \right\} \\ &\qquad -\tfrac{1}{2} G \textstyle\sum_{i \neq j} \left(\prod_{k \neq i, j} \delta_{n_{K_k}, n'_{K_k}} \delta_{n'_{L_k}, n_{L_k}} \right) \\ &\qquad \times \left\{ \left\langle n_{K_i}, n_{L_i} \left| \left(\hat{K}_i^+ + \hat{L}_i^+ \right) \right| n'_{K_i}, n'_{L_i} \right\rangle \left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^- + \hat{L}_j^- \right) \right| n'_{K_j}, n'_{L_j} \right\rangle \right. \\ &\qquad \left. + \left\langle n_{K_i}, n_{L_i} \left| \left(\hat{K}_i^- + \hat{L}_i^- \right) \right| n'_{K_i}, n'_{L_i} \right\rangle \left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^+ + \hat{L}_j^+ \right) \right| n'_{K_j}, n'_{L_j} \right\rangle \right\} \end{aligned}} \tag{B.27}$$

Using the matrix elements given by Eqs. (B.25), (B.26) and (B.27), the Hamiltonian matrix can be constructed and diagonalized with a standard numerical algorithm. The result is the spectrum of energies E_α of the many-body states $|\alpha\rangle$ along with their wave functions,

$$|\alpha\rangle = \sum_i C_i^\alpha \left| n_K^i, n_L^i \right\rangle \tag{B.28}$$

B.4 Transition Matrix Elements

Using Eqs. (B.4), (B.19) and (B.20) we can calculate the following matrix elements for the operator $\hat{D}_j$,

$$\left\langle n_{K_j}, n_{L_j} \left| \hat{D}_j \right| n'_{K_j}, n'_{L_j} \right\rangle = 2 \left(n_{K_j} - n_{L_j} \right) \delta_{n_{K_j}, n'_{K_j}} \delta_{n_{L_j}, n'_{L_j}} \tag{B.29}$$

from which we deduce the transition matrix element for the quadrupole operator $\hat{D}$ between many-body states $|\alpha\rangle$ and $|\beta\rangle$ given by Eq. (B.28) [4, 5],

$$\boxed{\left\langle \alpha \left| \hat{D} \right| \beta \right\rangle = 2 \sum_i \left(C_i^\alpha \right)^* C_i^\beta \sum_j d_j \left(n_{K_j}^i - n_{L_j}^i \right)} \tag{B.30}$$

B.5 Numerical Example and Discussion

We illustrate the formulas derived for the multi-O (4) with a numerical example taken from [3, 4]. In this example, $N = 28$ particles are distributed among three j shells with the properties given in Table B.1. The interaction strengths are $\chi = 0.04$ and $G = 0.14$. A total of 1894 basis states are generated by looping through all integer values of $n_{K_1}, n_{L_1}, n_{K_2}, n_{L_2}, n_{K_3}, n_{L_3}$ in the ranges $0 \leq n_{K_j}, n_{L_j} \leq \Omega_j/2$ and selecting those that satisfy $\sum_j \left(n_{K_j} + n_{L_j} \right) = N/2$=14.

Constructing the Hamiltonian matrix using Eqs. (B.25), (B.26) and (B.27) and diagonalizing it, the energies of the lowest 4 states are

$$E_0 = -16.944$$

$$E_1 = -16.853$$

$$E_2 = -15.338$$

$$E_3 = -14.767$$

and the transition matrix elements calculated using Eq. (B.30) are

$$\left\langle 0 \left| \hat{D} \right| 3 \right\rangle = 4.146$$

$$\left\langle 2 \left| \hat{D} \right| 3 \right\rangle = 21.441$$

$$\left\langle 1 \left| \hat{D} \right| 2 \right\rangle = 10.328$$

$$\left\langle 0 \left| \hat{D} \right| 1 \right\rangle = 27.824$$

in agreement with the numbers listed in Fig. 5 in [3] and Fig. 7 in [4].

Table B.1 Properties of the j shells for the numerical example

Shell no.	j	Ω_j	e_j^0	d_j
1	$\frac{27}{2}$	14	0.0	2.0
2	$\frac{19}{2}$	10	1.0	1.0
3	$\frac{7}{2}$	4	3.5	1.0

From Eq. (B.29) we see that the basis states in Eq. (B.17) are eigenstates of the quadrupole operator $\hat{D}$,

$$\hat{D} \left| n_K, n_L \right\rangle = \left[2 \sum_j d_j \left(n_{K_j} - n_{L_j} \right) \right] \left| n_K, n_L \right\rangle$$
$$\equiv D \left(n_K, n_L \right) \left| n_K, n_L \right\rangle$$

Thus, for the many-body state in Eq. (B.28) we can calculate a probability weight $P\left(D_0\right)$ for a given value $D\left(n_K, n_L\right) = D_0$,

$$P\left(D_0\right) = \sum_i \left| C_i^\alpha \right|^2 \delta_{D\left(n_K^i, n_L^i\right), D_0} \tag{B.31}$$

These probabilities are plotted in Fig. B.1 for the first few levels in the numerical example. We note for example that ground-state and first excited state have distributions peaked at $D_0 = \pm 32$, even though the overall expectation value for $\hat{D}$ for both levels can be calculated to be zero. In effect, the system in its ground state can be found in both $D_0 = +32$ and -32 states with equal probability, hence this is a case of strong shape mixing/coexistence between the two deformations.

These results can also be understood in the context of a microscopic approach starting from a mean-field approximation. The strong mixing between different deformations implies the existence of several local minima in the Hartree-Fock-Bogoliubov energy surface with respect to the deformation D_0, and that these minima are connected by a large-amplitude collective motion of the system. The theoretical tools we will apply to describe this behavior in the next sections can

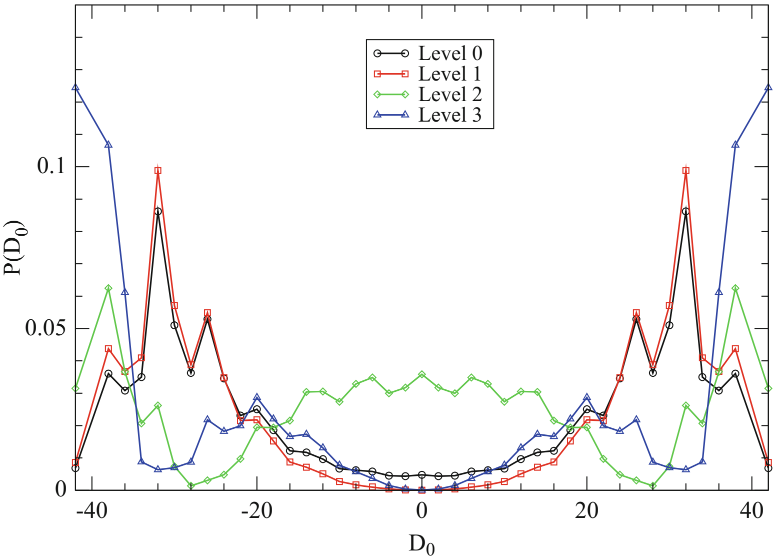

Fig. B.1 Probability weights $P(D_0)$ as a function of D_0 calculated using Eq. (B.31) for the numerical example

also be applied to the problem of fission, which shares some similarities with the phenomenon of shape coexistence.

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Appendix C
Projection on Particle Number

For additional discussions of particle-number projection, see for example [1–3].

C.1 Different Formulations of the Bogoliubov Vacuum

We recall the different ways of writing the Bogoliubov vacuum $\left|\tilde{0}\right\rangle$ that will be useful in the derivations that follow. First, we write the (unnormalized) vacuum in terms of quasiparticle destruction operators acting on the particle vacuum, $|0\rangle$,

$$\left|\tilde{0}\right\rangle = \prod_{\mu} \eta_{\mu} \, |0\rangle$$

We may also write the vacuum in the canonical basis (e.g., section 7.2.1 in [1]),

$$\alpha_{\mu}^{\dagger} = u_{\mu} a_{\mu}^{\dagger} - v_{\mu} a_{\bar{\mu}}$$
$$\alpha_{\bar{\mu}}^{\dagger} = u_{\mu} a_{\bar{\mu}}^{\dagger} + v_{\mu} a_{\mu}$$

where the canonical particle operators $\left(a_{\mu}^{\dagger}, a_{\bar{\mu}}^{\dagger}\right)$ are related to the "usual" particle operators in Eq. (1.1) by a unitary transformation, and likewise the canonical qp operators $\left(\alpha_{\mu}^{\dagger}, \alpha_{\bar{\mu}}^{\dagger}\right)$ in that same equation by another unitary transformation. Then, it can be shown that [1]

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$$\left|\tilde{0}\right\rangle = \exp\left[\sum_{\mu>0}\theta_\mu\left(a^\dagger_\mu a^\dagger_{\bar{\mu}} + a_\mu a_{\bar{\mu}}\right)\right]|0\rangle$$
$$= \left(\prod_{\mu>0} u_\mu\right)\exp\left[\sum_{\mu>0}\tan\theta_\mu a^\dagger_\mu a^\dagger_{\bar{\mu}}\right]|0\rangle$$

where we have defined

$$\tan\theta_\mu \equiv \frac{v_\mu}{u_\mu} \tag{C.1}$$

This can also be written as

$$\left|\tilde{0}\right\rangle = \left(\prod_{\mu>0} u_\mu\right)\prod_{\mu>0}\left(1 + \tan\theta_\mu a^\dagger_\mu a^\dagger_{\bar{\mu}}\right)|0\rangle \tag{C.2}$$

or

$$\left|\tilde{0}\right\rangle = \prod_{\mu>0}\left(u_\mu + v_\mu a^\dagger_\mu a^\dagger_{\bar{\mu}}\right)|0\rangle \tag{C.3}$$

In all its forms, the vacuum satisfies

$$\eta_\mu\left|\tilde{0}\right\rangle = \alpha_\mu\left|\tilde{0}\right\rangle = 0$$

C.2 A “Pedestrian” Approach

We choose the expression in Eq. (C.2) of the vacuum that we express in the more compact form

$$\left|\tilde{0}\right\rangle = \left(\prod_{\mu>0} u_\mu\right)\prod_{\mu>0}\left(1 + \hat{t}_\mu\right)|0\rangle \tag{C.4}$$

where

$$\hat{t}_\mu \equiv \tan\theta_\mu a^\dagger_\mu a^\dagger_{\bar{\mu}}$$

and where we have

$$\left[\hat{t}_\mu, \hat{t}_\nu\right] = 0 \tag{C.5}$$

The operators $\hat{t}_\mu$ create a pair of nucleons $(\mu, \bar{\mu})$. By expanding the product in Eq. (C.4) it is straightforward to project out the contribution of a number p of pairs to the vacuum defined in Eq. (C.2). If we define the (even) number of particles N as $N = 2p$, then the state with the correct number of particles N is given by the expression

$$|(p)\rangle = \left(\prod_{\mu>0} u_\mu\right) \sum_{0<\mu_1<\mu_2<\ldots<\mu_p} \hat{t}_{\mu_1}\hat{t}_{\mu_2}\ldots\hat{t}_{\mu_p}\,|0\rangle \tag{C.6}$$

In what follows, for the sake of simplicity we do not write the normalization factor $\left(\prod_{\mu>0} u_\mu\right)$ explicitly unless it is necessary. Note that Eq. (C.6) does not take into account the dimension D of the particle basis. In practice, the indices μ_i in Eq. (C.6) should satisfy

$$\mu_1 \leq D - p + 1,\ \ \mu_2 \leq D - p + 2, \ldots,\ \ \mu_p \leq D \tag{C.7}$$

For practical reasons, as we will see later, it is convenient to introduce an equivalent form which has the advantage of being symmetric,

$$|(p)\rangle = \frac{1}{p!} \sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_p} \hat{t}_{\mu_1}\hat{t}_{\mu_2}\ldots\hat{t}_{\mu_p}\,|0\rangle \tag{C.8}$$

with the further restrictions on the indices,

$$0 < \mu_i \leq D,\ \ i = 1, 2, \ldots, p \tag{C.9}$$

C.2.1 Illustration with a Simple Example

To illustrate these results, we consider a simple system with $N = 6$ particles (i.e., $p = 3$ pairs) in 4 doubly degenerate levels labeled 1, 2, 3, 4. We write the corresponding state according to Eq. (C.8),

$$\begin{aligned}
|(3)\rangle = \frac{1}{3!}\Big\{ & \hat{t}_1\hat{t}_2\hat{t}_3 + \hat{t}_1\hat{t}_3\hat{t}_2 + \hat{t}_2\hat{t}_1\hat{t}_3 + \hat{t}_2\hat{t}_3\hat{t}_1 + \hat{t}_3\hat{t}_1\hat{t}_2 + \hat{t}_3\hat{t}_2\hat{t}_1 \\
& + \hat{t}_1\hat{t}_2\hat{t}_4 + \hat{t}_1\hat{t}_4\hat{t}_2 + \hat{t}_2\hat{t}_1\hat{t}_4 + \hat{t}_2\hat{t}_4\hat{t}_1 + \hat{t}_4\hat{t}_1\hat{t}_2 + \hat{t}_4\hat{t}_2\hat{t}_1 \\
& + \hat{t}_1\hat{t}_3\hat{t}_4 + \hat{t}_1\hat{t}_4\hat{t}_3 + \hat{t}_3\hat{t}_1\hat{t}_4 + \hat{t}_3\hat{t}_4\hat{t}_1 + \hat{t}_4\hat{t}_1\hat{t}_3 + \hat{t}_4\hat{t}_3\hat{t}_1 \\
& + \hat{t}_2\hat{t}_3\hat{t}_4 + \hat{t}_2\hat{t}_4\hat{t}_3 + \hat{t}_3\hat{t}_2\hat{t}_4 + \hat{t}_3\hat{t}_4\hat{t}_2 + \hat{t}_4\hat{t}_2\hat{t}_3 + \hat{t}_4\hat{t}_3\hat{t}_2 \Big\}\,|0\rangle
\end{aligned} \tag{C.10}$$

We can also use Eq. (C.5) to reorder and combine terms in Eq. (C.10) to recover the form in Eq. (C.6),

$$|(3)\rangle = \left(\hat{t}_1\hat{t}_2\hat{t}_3 + \hat{t}_1\hat{t}_2\hat{t}_4 + \hat{t}_1\hat{t}_3\hat{t}_4 + \hat{t}_2\hat{t}_3\hat{t}_4\right)|0\rangle \tag{C.11}$$

In later calculations in this appendix we will need numerical values for the occupation probabilities, for which we take

$$v_1^2 = 0.9, \quad v_2^2 = 0.6, \quad v_3^2 = 0.4, \quad v_4^2 = 0.1$$

C.2.2 Normalization

First we can show by Wick's theorem that

$$\begin{aligned} &\sum_{\substack{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_p \\ \mu'_1 \neq \mu'_2 \neq \ldots \neq \mu'_p}} \left\langle 0 \left| \hat{t}^\dagger_{\mu'_1}\hat{t}^\dagger_{\mu'_2}\ldots\hat{t}^\dagger_{\mu'_p}\hat{t}_{\mu_1}\hat{t}_{\mu_2}\ldots\hat{t}_{\mu_p}\right| 0\right\rangle \\ &= p! \sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_p} \left(\tan\theta_{\mu_1}\tan\theta_{\mu_2}\ldots\tan\theta_{\mu_p}\right)^2 \end{aligned} \tag{C.12}$$

Then, starting from Eq. (C.8) and re-introducing the normalization of the state, the calculation of the norm is straightforward giving

$$\langle(p)|(p)\rangle = \frac{\left(\prod_{\mu=1}^{D} u_\mu^2\right)}{p!} \sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_p} \left(\tan\theta_{\mu_1}\tan\theta_{\mu_2}\ldots\tan\theta_{\mu_p}\right)^2 \tag{C.13}$$

with the restrictions on the indices given in Eq. (C.9). Similarly, Eq. (C.6) or (C.8) yields

$$\langle(p)|(p)\rangle = \left(\prod_{\mu=1}^{D} u_\mu^2\right) \sum_{0<\mu_1<\mu_2<\ldots<\mu_p} \left(\tan\theta_{\mu_1}\tan\theta_{\mu_2}\ldots\tan\theta_{\mu_p}\right)^2 \tag{C.14}$$

with the restrictions on the indices given by Eq. (C.7). Notice that using Eq. (C.1), we could also write these as

$$\langle(p)|(p)\rangle = \sum_{0<\mu_1<\mu_2<\ldots<\mu_p} \left(\prod_{\nu=\mu_{p+1}}^{D} u_\nu^2\right) \left(v_{\mu_1}v_{\mu_2}\ldots v_{\mu_p}\right)^2 \tag{C.15}$$

or

$$\langle (p)|\,(p)\rangle = \frac{1}{p!} \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_p} \left(\prod_{\nu=\mu_{p+1}}^{D} u_\nu^2 \right) \left(v_{\mu_1} v_{\mu_2} \ldots v_{\mu_p} \right)^2 \tag{C.16}$$

In the formalism of [4], this normalization is denoted as

$$\langle (p)|\,(p)\rangle = R_0^0 \tag{C.17}$$

In the expansion of Eq. (C.15) or (C.16) it is clear that each term is the probability to find a Slater determinant with N particles, and their sum $\langle (p)|\,(p)\rangle = R_0^0$ can then be interpreted as the overall probability to find N particles in the BCS vacuum.

C.2.3 One-Body Density Matrix

Next we consider the matrix elements $\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle$. For this calculation, Eq. (C.8) is the most convenient and we get (using $\left[a_\mu^\dagger a_\mu, a_\nu^\dagger a_{\bar{\nu}}^\dagger \right] = \delta_{\mu\nu} a_\nu^\dagger a_{\bar{\nu}}^\dagger$)

$$a_\mu^\dagger a_\mu \,|(p)\rangle = \frac{\hat{t}_\mu}{(p-1)!} \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_{p-1};\, \mu_i \neq \mu} \hat{t}_{\mu_1} \hat{t}_{\mu_2} \ldots \hat{t}_{\mu_{p-1}} \,|0\rangle \tag{C.18}$$

where the notation indicates that the state μ is to be taken out of all the summations, and where we have the further restrictions

$$0 < \mu_i \leq D, \; i = 1, 2, \ldots, p-1$$

We can illustrate this result with the simple example in Sect. C.2.1. Thus starting from Eq. (C.10), we have for example

$$\begin{aligned} a_2^\dagger a_2 \,|(3)\rangle = \frac{1}{3!} \{ & \hat{t}_1 \hat{t}_2 \hat{t}_3 + \hat{t}_1 \hat{t}_3 \hat{t}_2 + \hat{t}_2 \hat{t}_1 \hat{t}_3 + \hat{t}_2 \hat{t}_3 \hat{t}_1 + \hat{t}_3 \hat{t}_1 \hat{t}_2 + \hat{t}_3 \hat{t}_2 \hat{t}_1 \\ & + \hat{t}_1 \hat{t}_2 \hat{t}_4 + \hat{t}_1 \hat{t}_4 \hat{t}_2 + \hat{t}_2 \hat{t}_1 \hat{t}_4 + \hat{t}_2 \hat{t}_4 \hat{t}_1 + \hat{t}_4 \hat{t}_1 \hat{t}_2 + \hat{t}_4 \hat{t}_2 \hat{t}_1 \\ & + \hat{t}_2 \hat{t}_3 \hat{t}_4 + \hat{t}_2 \hat{t}_4 \hat{t}_3 + \hat{t}_3 \hat{t}_2 \hat{t}_4 + \hat{t}_3 \hat{t}_4 \hat{t}_2 + \hat{t}_4 \hat{t}_2 \hat{t}_3 + \hat{t}_4 \hat{t}_3 \hat{t}_2 \} \,|0\rangle \end{aligned}$$

where we used $\left[a_\mu^\dagger a_\mu, a_\nu^\dagger a_{\bar{\nu}}^\dagger \right] = \delta_{\mu\nu} a_\nu^\dagger a_{\bar{\nu}}^\dagger$. Then, factoring out $\hat{t}_2$ and combining like terms,

$$
\begin{aligned}
a_2^\dagger a_2 \left|(3)\right\rangle &= \frac{\hat{t}_2}{3!}\left(3\hat{t}_1\hat{t}_3 + 3\hat{t}_3\hat{t}_1 + 3\hat{t}_1\hat{t}_4 + 3\hat{t}_4\hat{t}_1 + 3\hat{t}_3\hat{t}_4 + 3\hat{t}_4\hat{t}_3\right)\left|0\right\rangle \\
&= \frac{\hat{t}_2}{2!}\left(\hat{t}_1\hat{t}_3 + \hat{t}_3\hat{t}_1 + \hat{t}_1\hat{t}_4 + \hat{t}_4\hat{t}_1 + \hat{t}_3\hat{t}_4 + \hat{t}_4\hat{t}_3\right)\left|0\right\rangle
\end{aligned} \tag{C.19}
$$

which is just what Eq. (C.18) predicts. We can also show that

$$
a_{\bar{\mu}}^\dagger a_{\bar{\mu}} \left|(p)\right\rangle = a_\mu^\dagger a_\mu \left|(p)\right\rangle \tag{C.20}
$$

Now taking the scalar product with the projected state $|(p)\rangle$ and using Eq. (C.12) we find

$$
\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{\tan^2\theta_\mu}{(p-1)!} \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_{p-1};\, \mu_i \neq \mu} \left(\tan\theta_{\mu_1}\tan\theta_{\mu_2}\ldots\tan\theta_{\mu_{p-1}}\right)^2 \tag{C.21}
$$

with

$$
0 < \mu_i \leq D,\ i = 1, 2, \ldots, p-1
$$

We can also write this as

$$
\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \tan^2\theta_\mu \sum_{\mu_1 < \mu_2 < \ldots < \mu_{p-1};\, \mu_i \neq \mu} \left(\tan\theta_{\mu_1}\tan\theta_{\mu_2}\ldots\tan\theta_{\mu_{p-1}}\right)^2 \tag{C.22}
$$

with the restrictions

$$
0 < \mu_1 \leq D - p + 1,\ 0 < \mu_2 \leq D - p + 2, \ldots,\ 0 < \mu_{p-1} \leq D
$$

After inserting the normalization, we obtain

$$
\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{(p-1)!} \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_{p-1};\, \mu_i \neq \mu} \left(\prod_{\nu=\mu_p}^{\mu_D} u_\nu^2\right) \left(v_{\mu_1} v_{\mu_2} \ldots v_{\mu_{p-1}}\right)^2
$$

or

$$
\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = v_\mu^2 \sum_{\mu_1 < \mu_2 < \ldots < \mu_{p-1};\, \mu_i \neq \mu} \left(\prod_{\nu=\mu_p}^{\mu_D} u_\nu^2\right) \left(v_{\mu_1} v_{\mu_2} \ldots v_{\mu_{p-1}}\right)^2 \tag{C.23}
$$

This is simply related to the quantity $R_1^1(\mu)$ defined in the residue approach of Dietrich et al. [4] through the relation

$$
\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = v_\mu^2 R_1^1(\mu) \tag{C.24}
$$

We can use the 4-level example in Sect. C.2.1 to illustrate these results by calculating $\left\langle (3) \left| a_2^\dagger a_2 \right| (3) \right\rangle$ either by taking the overlap of the states in Eqs. (C.19) and (C.11) and explicitly evaluating the Wick's contractions, or by applying Eq. (C.22). In either case we find

$$\left\langle (3) \left| a_2^\dagger a_2 \right| (3) \right\rangle = \tan^2\theta_2 \left(\tan^2\theta_1 \tan^2\theta_3 + \tan^2\theta_1 \tan^2\theta_4 + \tan^2\theta_3 \tan^2\theta_4 \right)$$

Including the normalization, this becomes

$$\left\langle (3) \left| a_2^\dagger a_2 \right| (3) \right\rangle = v_2^2 \left(u_4^2 v_1^2 v_3^3 + u_3^2 v_1^2 v_4^3 + u_1^2 v_3^2 v_4^3 \right)$$

C.2.4 Two-Body Density Matrix

We will first calculate (for $\mu \neq \nu$)

$$\left\langle (p) \left| a_\mu^\dagger a_\nu^\dagger a_\nu a_\mu \right| (p) \right\rangle = \left\langle (p) \left| a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu \right| (p) \right\rangle$$

Starting from Eq. (C.18) we find

$$a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu \left| (p) \right\rangle = \frac{\hat{t}_\nu \hat{t}_\mu}{(p-2)!} \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_{p-2}; \{\mu_i \neq \mu, \nu\}} \hat{t}_{\mu_1} \hat{t}_{\mu_2} \ldots \hat{t}_{\mu_{p-2}} \left| 0 \right\rangle$$

with

$$0 < \mu_i \leq D, \; i = 1, 2, \ldots, p-2$$

which leads to

$$\left\langle (p) \left| a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{\left(\tan\theta_\mu \tan\theta_\nu \right)^2}{(p-2)!} \times \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_{p-2}; \{\mu_i \neq \mu, \nu\}} \left(\tan\theta_1 \tan\theta_2 \ldots \tan\theta_{p-2} \right)^2$$

with the restrictions stated above,

$$0 < \mu_i \leq D, \; i = 1, 2, \ldots, p-2$$

or, if we order the indices,

$$\left\langle (p) \left| a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu \right| (p) \right\rangle = \left(\tan\theta_\mu \tan\theta_\nu\right)^2 \times \sum_{\mu_1<\mu_2<\ldots<\mu_{p-2};\{\mu_i\neq\mu,\nu\}} \left(\tan\theta_1 \tan\theta_2 \ldots \tan\theta_{p-2}\right)^2 \tag{C.25}$$

Again, if we multiply by the normalization, the correct form is

$$\left\langle (p) \left| a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu \right| (p) \right\rangle = \left(v_\mu v_\nu\right)^2 \sum_{\mu_1<\mu_2<\ldots<\mu_{p-2};\{\mu_i\neq\mu,\nu\}} \left(\prod_{\substack{\alpha=\mu_{p-1} \\ \alpha\neq\mu,\nu}}^{\mu_D} u_\alpha^2 \right) \times \left(v_1 v_2 \ldots v_{p-2}\right)^2$$

which we can relate to the $R_2^2(\mu,\nu)$ of Dietrich et al. [4] by

$$\left\langle (p) \left| a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu \right| (p) \right\rangle = R_2^2(\mu,\nu)\left(v_\mu v_\nu\right)^2 \tag{C.26}$$

We illustrate this result with the 4-level example of Sect. C.2.1 by first applying $a_3^\dagger a_3$ to Eq. (C.19) to obtain

$$a_3^\dagger a_3 a_2^\dagger a_2 \left|(3)\right\rangle = \frac{\hat{t}_3 \hat{t}_2}{1!}\left(\hat{t}_1 + \hat{t}_4\right)\left|0\right\rangle$$

Then, taking the dot product with Eq. (C.11) we get

$$\begin{aligned}\left\langle (p) \left| a_3^\dagger a_3 a_2^\dagger a_2 \right| (p) \right\rangle &= \left\langle (p) \left| \hat{t}_3^\dagger \hat{t}_2^\dagger \hat{t}_1^\dagger \hat{t}_1 \hat{t}_2 \hat{t}_3 + \hat{t}_4^\dagger \hat{t}_3^\dagger \hat{t}_2^\dagger \hat{t}_2 \hat{t}_3 \hat{t}_4 \right| (p) \right\rangle \\ &= \tan^2\theta_2 \tan^2\theta_3 \left(\tan^2\theta_1 + \tan^2\theta_4\right)\end{aligned}$$

which we can also obtain directly from Eq. (C.25).

As we shall see in Sect. C.2.5, we also need to calculate the matrix elements $\left\langle (p) \left| a_\mu^\dagger a_{\bar\mu}^\dagger a_{\bar\nu} a_\nu \right| (p) \right\rangle$. For this, we can use Eq. (C.8) and the commutator

$$\left[a_{\bar\nu} a_\nu, a_\mu^\dagger a_{\bar\mu}^\dagger\right] = \delta_{\mu\nu}\left(1 - a_\mu^\dagger a_\nu - a_{\bar\mu}^\dagger a_{\bar\nu}\right)$$

to calculate

$$a_{\bar\nu} a_\nu \left|(p)\right\rangle = \frac{\tan\theta_\nu}{(p-1)!} \sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_{p-1};\{\mu_i\neq\nu\}} \hat{t}_{\mu_1} \hat{t}_{\mu_2} \ldots \hat{t}_{\mu_{p-1}} \left|0\right\rangle$$

and

$$\langle (p)|\, a_{\mu}^{\dagger} a_{\bar{\mu}}^{\dagger} = \frac{\tan\theta_{\mu}}{(p-1)!}\, \langle 0| \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_{p-1}; \{\mu_i \neq \mu\}} \hat{t}_{\mu_{p-1}}^{\dagger} \ldots \hat{t}_{\mu_2}^{\dagger} \hat{t}_{\mu_1}^{\dagger}$$

with the usual restrictions

$$0 < \mu_i \leq D,\ i = 1, 2, \ldots, p-1$$

The desired matrix element is obtained by taking the scalar product which leads to

$$\left\langle (p) \left| a_{\mu}^{\dagger} a_{\bar{\mu}}^{\dagger} a_{\bar{\nu}} a_{\nu} \right| (p) \right\rangle = \frac{\tan\theta_{\mu} \tan\theta_{\nu}}{(p-1)!} \times \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_{p-1}; \{\mu_i \neq \mu, \nu\}} \left(\tan\theta_1 \tan\theta_2 \ldots \tan\theta_{p-1}\right)^2 \tag{C.27}$$

After taking care of the normalization, this gives

$$\left\langle (p) \left| a_{\mu}^{\dagger} a_{\bar{\mu}}^{\dagger} a_{\bar{\nu}} a_{\nu} \right| (p) \right\rangle = u_{\mu} v_{\mu} u_{\nu} v_{\nu} \sum_{\mu_1 < \mu_2 < \ldots < \mu_{p-1}; \{\mu_i \neq \mu, \nu\}} \left(\prod_{\substack{\alpha = \mu_p \\ \alpha \neq \mu, \nu}}^{\mu_D} u_{\alpha}^2 \right) \times \left(v_1 v_2 \ldots v_{p-1}\right)^2$$

which is related to the coefficient defined by Dietrich et al. [4] through

$$\left\langle (p) \left| a_{\mu}^{\dagger} a_{\bar{\mu}}^{\dagger} a_{\bar{\nu}} a_{\nu} \right| (p) \right\rangle = u_{\mu} v_{\mu} u_{\nu} v_{\nu} R_1^2 (\mu, \nu) \tag{C.28}$$

We illustrate this result with the 4-level example by calculating $\left\langle (p) \left| a_3^{\dagger} a_{\bar{3}}^{\dagger} a_{\bar{2}} a_2 \right| (p) \right\rangle$. From Eq. (C.11), we first calculate

$$a_{\bar{2}} a_2 \,|(3)\rangle = \tan\theta_2 \left(\hat{t}_1 \hat{t}_3 + \hat{t}_1 \hat{t}_4 + \hat{t}_3 \hat{t}_4\right) |0\rangle$$

and similarly,

$$a_{\bar{3}} a_3 \,|(3)\rangle = \tan\theta_3 \left(\hat{t}_1 \hat{t}_2 + \hat{t}_1 \hat{t}_4 + \hat{t}_2 \hat{t}_4\right) |0\rangle$$

and taking the scalar product,

$$\left\langle (p) \left| a_3^{\dagger} a_{\bar{3}}^{\dagger} a_{\bar{2}} a_2 \right| (p) \right\rangle = \tan\theta_2 \tan\theta_3 \left(\tan^2\theta_1 \tan^2\theta_4\right)$$

which we can also get directly from Eq. (C.27).

C.2.5 Projected Expectation Value of the Two-Body Potential

We now wish to calculate

$$V(p) \equiv \frac{1}{4} \sum_{\mu_1,\mu_2,\mu_3,\mu_4} \langle \mu_1, \mu_2 | V | \widetilde{\mu_3, \mu_4} \rangle \left\langle (p) \left| a^\dagger_{\mu_1} a^\dagger_{\mu_2} a_{\mu_4} a_{\mu_3} \right| (p) \right\rangle$$

where the notation $\left|\widetilde{\mu_3, \mu_4}\right\rangle \equiv |\mu_3, \mu_4\rangle - |\mu_4, \mu_3\rangle$ serves as a reminder that the matrix elements of V are anti-symmetrized. The summation indices $(\mu_1, \mu_2, \mu_3, \mu_4)$ are not independent, but must be chosen such that the four operators conserve the number of pairs when applied to the projected state $|(p)\rangle$. This condition is satisfied only by combinations of the type

$$a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu, \quad a^\dagger_\mu a^\dagger_{\bar{\mu}} a_{\bar{\nu}} a_\nu$$

Thus we will write

$$\begin{aligned} V(p) &= \frac{1}{4} \sum_{\mu,\nu} \langle \mu, \nu | V | \widetilde{\mu, \nu} \rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p) \right\rangle \\ &+ \frac{1}{4} \sum_{\mu,\nu} \langle \mu, \bar{\mu} | V | \widetilde{\nu, \bar{\nu}} \rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar{\mu}} a_{\bar{\nu}} a_\nu \right| (p) \right\rangle \end{aligned} \tag{C.29}$$

We take into account the fact that the indices run over positive $(\mu, \nu > 0)$ and negative $(\bar{\mu}, \bar{\nu})$ values and that we have time-reversal invariance. In particular, we have the following properties under action of the time-reversal operator $\hat{K}$ (and choosing a representation where all the matrix elements are real),

$$\begin{aligned} \langle \bar{\mu}, \bar{\nu} | V | \bar{\mu}, \bar{\nu} \rangle &= \left(\langle \bar{\mu}, \bar{\nu} | \hat{K} \right) V \left(\hat{K} | \bar{\mu}, \bar{\nu} \rangle \right) \\ &= \left\langle \mu, \nu \left| \hat{K}^\dagger V \hat{K} \right| \mu, \nu \right\rangle^* \\ &= \langle \mu, \nu | V | \mu, \nu \rangle^* \\ &= \langle \mu, \nu | V | \mu, \nu \rangle \end{aligned}$$

and also,

$$\hat{K} |(p)\rangle = |(p)\rangle$$

As a result,

$$\left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p) \right\rangle = \left\langle (p) \left| a^\dagger_{\bar\mu} a^\dagger_{\bar\nu} a_{\bar\nu} a_{\bar\mu} \right| (p) \right\rangle$$

and

$$\left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar\mu} a_{\bar\nu} a_\nu \right| (p) \right\rangle = \left\langle (p) \left| a^\dagger_{\bar\mu} a^\dagger_\mu a_\nu a_{\bar\nu} \right| (p) \right\rangle$$

Let us now consider the first term in Eq. (C.29). The summation in this term can be expanded as

$$\sum_{\mu,\nu} = \sum_{\mu>0,\nu>0} + \sum_{\mu<0,\nu<0} + \sum_{\mu>0,\nu<0} + \sum_{\mu<0,\nu>0}$$

and according to the properties under time reversal demonstrated above, this term reduces to

$$\begin{aligned}
&\frac{1}{4}\sum_{\mu,\nu} \langle \mu, \nu \,|V|\, \widetilde{\mu, \nu} \rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p) \right\rangle \\
&\quad = \frac{1}{2}\sum_{\mu,\nu>0} \Big(\langle \mu, \nu \,|V|\, \widetilde{\mu, \nu} \rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p) \right\rangle \\
&\qquad \langle \mu, \bar\nu \,|V|\, \widetilde{\mu, \bar\nu} \rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar\nu} a_{\bar\nu} a_\mu \right| (p) \right\rangle \Big)
\end{aligned}$$

Referring back to Eq. (C.20) it is clear that

$$\left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p) \right\rangle = \left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar\nu} a_{\bar\nu} a_\mu \right| (p) \right\rangle$$

and therefore we finally obtain

$$\begin{aligned}
&\frac{1}{4}\sum_{\mu,\nu} \langle \mu, \nu \,|V|\, \widetilde{\mu, \nu} \rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p) \right\rangle \\
&\quad = \frac{1}{2}\sum_{\mu,\nu>0} \left(\langle \mu, \nu \,|V|\, \widetilde{\mu, \nu} \rangle + \langle \mu, \bar\nu \,|V|\, \widetilde{\mu, \bar\nu} \rangle \right) \\
&\qquad \times \left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p) \right\rangle
\end{aligned}$$

By proceeding in a similar manner, the second term in Eq. (C.29) takes the form

$$\frac{1}{4}\sum_{\mu,\nu} \langle \mu, \bar\mu \,|V|\, \widetilde{\nu, \bar\nu} \rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar\mu} a_{\bar\nu} a_\nu \right| (p) \right\rangle = \sum_{\mu,\nu>0} \langle \mu, \bar\mu \,|V|\, \widetilde{\nu, \bar\nu} \rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar\mu} a_{\bar\nu} a_\nu \right| (p) \right\rangle$$

Finally, the projected expectation value of the energy takes the form

$$\frac{\left\langle (p) \left| \hat{H} \right| (p) \right\rangle}{\langle (p) | (p) \rangle} = \frac{1}{R_0^0} \Bigg\{ 2 \sum_{\mu>0} \left\langle \mu \left| \hat{T} \right| \mu \right\rangle R_1^1 (\mu) v_\mu^2 + \frac{1}{2} \sum_{\mu,\nu>0} \left(\langle \mu, \nu | V | \widetilde{\mu, \nu} \rangle + \langle \mu, \bar{\nu} | V | \widetilde{\mu, \bar{\nu}} \rangle \right) R_2^2 (\mu, \nu) \left(v_\mu v_\nu \right)^2 + \sum_{\mu,\nu>0} \langle \mu, \bar{\mu} | V | \widetilde{\nu, \bar{\nu}} \rangle R_1^2 (\mu, \nu) u_\mu v_\mu u_\nu v_\nu \Bigg\} \tag{C.30}$$

where we have used Eqs. (C.17), (C.24), (C.26), and (C.28).

This derivation concludes the pedestrian approach to particle-number projection. In principle, the expression in Eq. (C.30) can always be evaluated numerically, and there are recursion relations for the R_i^j coefficients [4]. In practice, these calculations can be cumbersome and time-consuming. Next, we examine the projector proposed by Dietrich et al. [4] as another way of enforcing particle-number conservation.

C.3 A Projection Operator on Particle Number

C.3.1 Basic Definitions

Let us first introduce the problem of projection with basic and straightforward definitions that will be useful in what follows. Clearly the problem arises when we use a description with an indefinite number of particles, and consequently it is important to define a complete set of states adapted to such a situation. We assume that we have a complete set of vectors to describe any system with a given number of particles. We denote by

$$\{|(i) , N\rangle\} \tag{C.31}$$

the basis for a system with N particles. More precisely, any wave function with N particles can be expanded as

$$|\Psi\rangle = \sum_i \langle (i) , N | \Psi \rangle \, |(i) , N\rangle$$

The expansion of a wave function with an indefinite number of particles is given by

$$|\Psi\rangle = \sum_{N,i} \langle (i), N | \Psi \rangle \, |(i), N\rangle$$

The closure relation or the identity operator in the Fock space reads

$$\hat{I} = \sum_{N,i} |(i), N\rangle \langle (i), N|$$

Now if $P^{(N)}$ is a projector in the N-particle space, it satisfies

$$P^{(N)} \left|(i), N'\right\rangle = \begin{cases} |(i), N\rangle & N' = N \\ 0 & N' \neq N \end{cases} \tag{C.32}$$

and consequently

$$P^{(N)} = P^{(N)} \hat{I} = \sum_{i} |(i), N\rangle \langle (i), N|$$

Thus we recover the well-known result that the closure relation in the N-space provides a representation of this projector. This expression is useful in the formalism, but not for practical applications. Therefore, we have to resort to other representations, one of them being the projector proposed by Dietrich et al. [4]. Its construction is straightforward thanks to the fact that the eigenvalues of the particle number operator are integers. In effect, to satisfy Eq. (C.32) we seek an operator that behaves like a Kronecker delta symbol when acting on the basis defined in Eq. (C.31). One such possible operator clearly is

$$P^{(N)} \equiv \frac{1}{2\pi} \int_0^{2\pi} d\varphi \, e^{i\varphi\left(\hat{N} - N\right)} \tag{C.33}$$

since

$$P^{(N)} \left|(i), N'\right\rangle = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \, e^{i\varphi(N' - N)} \left|(i), N'\right\rangle = \begin{cases} |(i), N\rangle & N' = N \\ 0 & N' \neq N \end{cases}$$

It is worth pointing out that the operator in Eq. (C.33) could also be written as

$$P^{(N)} = \frac{1}{2\pi} \int_\alpha^{2\pi + \alpha} d\varphi \, e^{i\varphi\left(\hat{N} - N\right)}$$

for an arbitrary real number α. This last remark is useful for certain demonstrations (e.g., that $P^{(N)\dagger} = P^{(N)}$, as expected).

C.3.2 Application

For practical applications, we re-write the operator of Eq. (C.33) in the form

$$P^{(N)} = \frac{1}{2\pi i} \oint dz \, \frac{z^{\hat{N}}}{z^{N+1}}, \qquad z = e^{i\varphi}$$

The integration contour is the unit circle. Let us now see the effect of this projector on a BCS state,

$$P^{(N)} \left|\mathrm{BCS}\right\rangle = \frac{1}{2\pi i} \oint dz \, \frac{z^{\hat{N}}}{z^{N+1}} \left|\mathrm{BCS}\right\rangle$$

To clarify the meaning of the operator $z^{\hat{N}}$ we go over to the exponential form

$$z^{\hat{N}} = e^{\hat{N} \ln z}$$

When applied to a pair state $a^\dagger_\mu a^\dagger_{\bar{\mu}} \left|0\right\rangle$ this operator gives

$$\begin{aligned} z^{\hat{N}} a^\dagger_\mu a^\dagger_{\bar{\mu}} \left|0\right\rangle &= e^{\hat{N} \ln z} a^\dagger_\mu a^\dagger_{\bar{\mu}} \left|0\right\rangle \\ &= e^{2 \ln z} a^\dagger_\mu a^\dagger_{\bar{\mu}} \left|0\right\rangle \\ &= z^2 a^\dagger_\mu a^\dagger_{\bar{\mu}} \left|0\right\rangle \end{aligned}$$

and therefore

$$P^{(N)} \left|\mathrm{BCS}\right\rangle = \frac{1}{2\pi i} \oint dz \, \frac{1}{z^{N+1}} \prod_{\mu>0} \left(u_\mu + z^2 v_\mu a^\dagger_\mu a^\dagger_{\bar{\mu}} \right) \left|0\right\rangle$$

If we set $N = 2p$ and $\varsigma = z^2$, we recover Eq. (2.3) in [4],

$$P^{(N)} \left|\mathrm{BCS}\right\rangle = C \oint d\varsigma \, \frac{1}{\varsigma^{p+1}} \prod_{\mu>0} \left(u_\mu + \varsigma v_\mu a^\dagger_\mu a^\dagger_{\bar{\mu}} \right) \left|0\right\rangle$$

with C a normalization constant. With this form of the projector it is clear that the integration picks out the coefficient of ς^p in the expansion of the product, that is, the component with p pairs. This is essentially what the pedestrian approach described above does. The same remark applies to the calculation of the one- and two-body matrices with this residue method.

C.4 Another Point of View

C.4.1 Alternate Form of the One-Body Density

We illustrate another way to use the Dietrich et al. projection operator described above by re-visiting the calculation of the one-body matrix elements. We could have chosen to start with the calculation of the projected norm, $\left\langle \text{BCS} \left| P^{(N)} \right| \text{BCS} \right\rangle$, but the one-body operator is a better choice to introduce some general techniques. The matrix elements of the one-body density operator calculated with the projected states can be written as

$$\begin{aligned} \left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle &= \left\langle \text{BCS} \left| a_\mu^\dagger a_\mu P^{(N=2p)} \right| \text{BCS} \right\rangle \\ &= \frac{1}{2\pi} \int_0^{2\pi} d\varphi\, e^{-i\varphi N} \left\langle \text{BCS} \left| a_\mu^\dagger a_\mu e^{i\hat{N}\varphi} \right| \text{BCS} \right\rangle \end{aligned} \tag{C.34}$$

Now instead of first projecting the BCS state and then calculating the matrix element as we did previously, we take out the integration and examine the quantity

$$\left\langle \text{BCS} \left| a_\mu^\dagger a_\mu e^{i\hat{N}\varphi} \right| \text{BCS} \right\rangle \tag{C.35}$$

Thanks to the simplicity of the particle operator, the calculation is straightforward. In effect, we introduce the quantity

$$\hat{\chi} \equiv e^{i\hat{N}\varphi} \tag{C.36}$$

with the properties

$$\hat{\chi}^\dagger \hat{\chi} = 1, \quad \hat{\chi}\,|0\rangle = |0\rangle \tag{C.37}$$

Furthermore, since we can readily show that $\left[\hat{N}, a^\dagger\right] = a^\dagger$ and $\left[\hat{N}, a\right] = -a$, it follows by the Baker-Campbell-Hausdorff relation that

$$\begin{aligned} \hat{\chi} a^\dagger \hat{\chi}^\dagger &= e^{i\varphi} a^\dagger \\ \hat{\chi} a \hat{\chi}^\dagger &= e^{-i\varphi} a \end{aligned}$$

and therefore,

$$\begin{aligned} \hat{\chi} a_\mu^\dagger a_{\bar{\mu}}^\dagger \hat{\chi}^\dagger &= \hat{\chi} a_\mu^\dagger \hat{\chi}^\dagger \hat{\chi} a_{\bar{\mu}}^\dagger \hat{\chi}^\dagger \\ &= e^{2i\varphi} a_\mu^\dagger a_{\bar{\mu}}^\dagger \end{aligned}$$

By applying the operator $\hat{\chi}$ and using the properties just given we easily obtain the transformed BCS state,

$$\begin{aligned} e^{i\hat{N}\varphi}|\mathrm{BCS}\rangle &= \hat{X}\left[\prod_{\mu>0}\left(u_\mu + v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger\right)\right]\hat{\chi}^\dagger\hat{\chi}|0\rangle \\ &= \prod_{\mu>0}\left[\hat{\chi}\left(u_\mu + v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger\right)\hat{\chi}^\dagger\right]|0\rangle \\ &= \prod_{\mu>0}\left(u_\mu + e^{2i\varphi}v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger\right)|0\rangle \\ &\equiv |\mathrm{BCS}(\varphi)\rangle \end{aligned} \tag{C.38}$$

As expected, the BCS state transformed with the $\hat{\chi}$ operator is still a BCS state. More generally, if we transform any Bogoliubov state

$$\left|\tilde{0}\right\rangle \equiv \prod_\mu \eta_\mu |0\rangle$$

with the operator $\hat{\chi}$, the transformed state is again a Bogoliubov vacuum of the quasiparticle destruction operators as defined below,

$$\begin{aligned} \eta_\mu \left|\tilde{0}\right\rangle &= 0 \\ \Rightarrow \hat{\chi}\eta_\mu\hat{\chi}^\dagger\hat{\chi}\left|\tilde{0}\right\rangle &= 0 \end{aligned}$$

which we can write as

$$\eta_\mu(\varphi)\left|\tilde{0}\right\rangle = 0$$

with

$$\begin{aligned} \eta_\mu(\varphi) &\equiv \hat{\chi}\eta_\mu\hat{\chi}^\dagger \\ &= \sum_{n>0}\left(u_{n\mu}\hat{\chi}a_n\hat{\chi}^\dagger - v_{n\mu}\hat{\chi}a_{\bar{n}}^\dagger\hat{\chi}^\dagger\right) \\ &= \sum_{n>0}\left(u_{n\mu}e^{-i\varphi}a_n - v_{n\mu}e^{i\varphi}a_{\bar{n}}^\dagger\right) \end{aligned}$$

and in the simple case of BCS quasiparticles, this reduces to

$$\eta_\mu(\varphi) = u_\mu e^{-i\varphi}a_\mu - v_\mu e^{i\varphi}a_{\bar{\mu}}^\dagger$$

and similarly,

$$\eta_{\bar{\mu}}(\varphi) = u_\mu e^{-i\varphi} a_{\bar{\mu}} + v_\mu e^{i\varphi} a_\mu^\dagger$$

Then we can calculate

$$\begin{aligned}
\left|\tilde{0}(\varphi)\right\rangle &= \prod_{\mu>0} \eta_\mu(\varphi)\,\eta_{\bar{\mu}}(\varphi)\,|0\rangle \\
&= \left(\prod_{\mu>0} v_\mu\right) \prod_{\mu>0} \left(u_\mu + e^{2i\varphi} v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger\right)|0\rangle \\
&= \left(\prod_{\mu>0} v_\mu\right) |\mathrm{BCS}(\varphi)\rangle
\end{aligned}$$

Note that this last expression contains the normalization of the state. We now have all the necessary ingredients to express Eq. (C.35) in the simple form

$$\begin{aligned}
\left\langle \mathrm{BCS}\left| a_\mu^\dagger a_\mu e^{i\hat{N}\varphi} \right| \mathrm{BCS}\right\rangle &= \left\langle 0 \left| \left[\prod_{\alpha>0}(u_\alpha + v_\alpha a_{\bar{\alpha}} a_\alpha)\right] a_\mu^\dagger a_\mu \right.\right. \\
&\quad \times \left.\left. \left[\prod_{\beta>0}\left(u_\beta + e^{2i\varphi} v_\beta a_\beta^\dagger a_{\bar{\beta}}^\dagger\right)\right] \right| 0 \right\rangle \\
&= \langle 0| \left[\prod_{\alpha>0}(u_\alpha + v_\alpha a_{\bar{\alpha}} a_\alpha)\right] \left[\prod_{\substack{\beta>0 \\ \beta\neq\mu}} \left(u_\beta + e^{2i\varphi} v_\beta a_\beta^\dagger a_{\bar{\beta}}^\dagger\right)\right] \\
&\quad \times \left[a_\mu^\dagger a_\mu, u_\mu + e^{2i\varphi} v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger\right]|0\rangle
\end{aligned}$$

where we have used the fact that $a_\mu^\dagger a_\mu$ commutes with all the terms $\left(u_\beta + e^{2i\varphi} v_\beta a_\beta^\dagger a_{\bar{\beta}}^\dagger\right)$ except when $\beta = \mu$ to introduce the commutator in the second line. Therefore

$$\left\langle \mathrm{BCS}\left| a_\mu^\dagger a_\mu e^{i\hat{N}\varphi} \right| \mathrm{BCS}\right\rangle = e^{2i\varphi} v_\mu^2 \left\langle \left| \left[\prod_{\substack{\alpha>0 \\ \alpha\neq\mu}} (u_\alpha + v_\alpha a_{\bar{\alpha}} a_\alpha)\right] \right.\right.$$

$$\times \left[\prod_{\substack{\beta > 0 \\ \beta \neq \mu}} \left(u_\beta + e^{2i\varphi} v_\beta a_\beta^\dagger a_{\bar{\beta}}^\dagger \right) \right] \Bigg| 0 \Big\rangle$$

$$= e^{2i\varphi} v_\mu^2 \prod_{\substack{\alpha > 0 \\ \alpha \neq \mu}} \left(u_\alpha^2 + e^{2i\varphi} v_\alpha^2 \right)$$

where the second line follows from a standard calculation of a BCS state norm. Inserting this into Eq. (C.34) we obtain finally

$$\Big\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \Big\rangle = \frac{v_\mu^2}{2\pi} \int_0^{2\pi} d\varphi \, e^{-i\varphi(N-2)} \prod_{\substack{\alpha > 0 \\ \alpha \neq \mu}} \left(u_\alpha^2 + e^{2i\varphi} v_\alpha^2 \right)$$

or, writing $N = 2p$ and making the substitution $2\varphi \to \varphi$, we get

$$\Big\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \Big\rangle = \frac{v_\mu^2}{2\pi} \int_0^{2\pi} d\varphi \, e^{-i\varphi(p-1)} \prod_{\substack{\alpha > 0 \\ \alpha \neq \mu}} \left(u_\alpha^2 + e^{i\varphi} v_\alpha^2 \right)$$

For numerical applications, it is convenient to re-write this integral in a different form. First, we write

$$u_\alpha^2 + e^{i\varphi} v_\alpha^2 = \left(1 - 2v_\alpha^2 \sin^2 \frac{\varphi}{2} \right) + i v_\alpha^2 \sin\varphi$$

and define the norm

$$\begin{aligned} n_\alpha(\varphi) &\equiv \left| u_\alpha^2 + e^{i\varphi} v_\alpha^2 \right| \\ &= \sqrt{1 - 4v_\alpha^2 \left(1 - v_\alpha^2\right) \sin^2 \frac{\varphi}{2}} \end{aligned}$$

and the argument[1]

[1]The notation $\tan^{-1}(x, y)$ refers to the arctangent, taking into account the quadrant that the point (x, y) is in.

$$\Omega_\alpha = \tan^{-1}\left(1 - 2v_\alpha^2 \sin^2 \frac{\varphi}{2}, v_\alpha^2 \sin\varphi\right)$$

This allows us to write the projected matrix element as

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{2\pi} \int_0^{2\pi} d\varphi \, e^{-i\left[\varphi(p-1) - \sum_{\alpha\neq\mu} \Omega_\alpha(\varphi)\right]} \prod_{\substack{\alpha>0 \\ \alpha\neq\mu}} n_\alpha(\varphi)$$

Taking into account the fact that the matrix element is real, this reduces to

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{2\pi} \int_0^{2\pi} d\varphi \, \cos\left[\sum_{\alpha\neq\mu} \Omega_\alpha(\varphi) - \varphi(p-1)\right] \prod_{\substack{\alpha>0 \\ \alpha\neq\mu}} n_\alpha(\varphi)$$

As a matter of convenience, we define the following quantities which are independent of μ,

$$n(\varphi) \equiv \prod_{\alpha>0} n_\alpha(\varphi)$$
$$\Omega(\varphi) \equiv \sum_{\alpha>0} \Omega_\alpha(\varphi)$$

and re-write the projected matrix element as

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{2\pi} \int_0^{2\pi} d\varphi \, \exp\left[\ln n(\varphi) - \ln n_\mu(\varphi)\right] \times \cos\left[\Omega(\varphi) - \Omega_\mu(\varphi) - \varphi(p-1)\right]$$

Finally by using the symmetry properties

$$n_\alpha(-\varphi) = n_\alpha(\varphi)$$
$$\Omega_\alpha(-\varphi) = -\Omega_\alpha(\varphi)$$

which follow straight from the definitions of n_α and Ω_α, and which also hold for the summed quantities $n(\varphi)$ and $\Omega(\varphi)$, we can reduce the domain of integration by half and write

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{\pi} \int_0^{\pi} d\varphi \, \exp\left[\ln n(\varphi) - \ln n_\mu(\varphi)\right] \times \cos\left[\Omega(\varphi) - \Omega_\mu(\varphi) - \varphi(p-1)\right]$$

Notice that all the quantities occurring in this expression are very simple to calculate. The only remaining problem is to evaluate the integral by an efficient method. Fortunately, these types of integrals have been considered in the literature (see, e.g., [5, 6] and section 11.4.3 in [1]), and it has been shown that they can be calculated by discretizing the angle φ as

$$\varphi_k = \frac{\pi k}{L}$$

over a small number of values $k = 0, 1, \ldots, L$. Note that the integrand is 1 when $\varphi = 0$ giving us the first integration point. In other words,

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle \approx \frac{v_\mu^2}{L} \sum_{k=0}^{L-1} \exp\left[\ln n(\varphi_k) - \ln n_\mu(\varphi_k)\right] \times \cos\left[\Omega(\varphi_k) - \Omega_\mu(\varphi_k) - \varphi_k(p-1)\right] \tag{C.39}$$

We show in Fig. C.1 the convergence of this quantity for the simple 4-level example described in Sect. C.2.1.

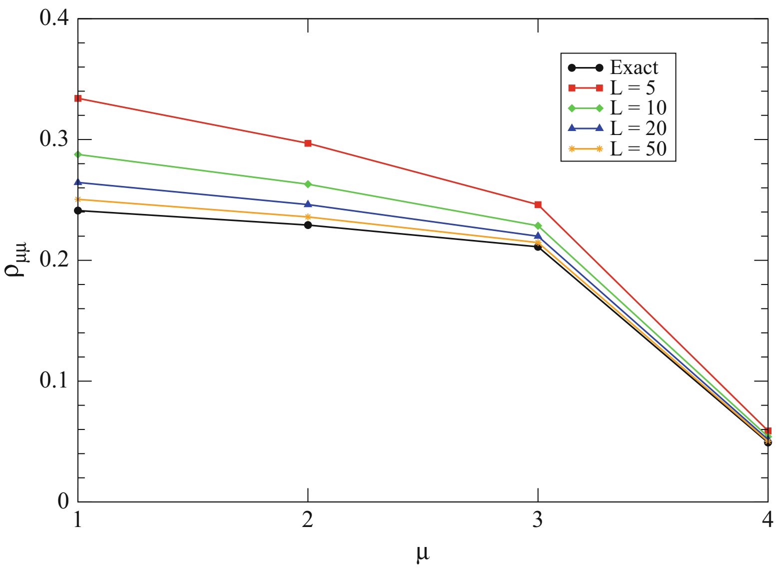

Fig. C.1 Plot of the density matrix elements $\rho_{\mu\mu} = \left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle$ as a function of state μ for the 4-level example of Sect. C.2.1. The curve labeled "Exact" corresponds the calculation using Eq. (C.23), the other curves were obtained using Eq. (C.39) for different number L of integration points

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Appendix D
Particle-Number Projected GCM Matrix Elements

D.1 General Results

In this appendix we derive expressions for particle-number projected matrix elements between BCS states at different deformation by combining the projection approach described in Sect. C.4 with the procedure developed in [1] to calculate non-diagonal matrix elements. In general, this will involve the calculation of matrix elements of the form

$$\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} \hat{O} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \, e^{-i(\varphi'-\varphi)N} \times \left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q \varphi} \hat{O} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle \tag{D.1}$$

for some operator $\hat{O}$ and where we have labeled the number operator and its corresponding projection operator by deformation parameters q and q' as a reminder that the operators are expanded on a basis which may vary as a function of deformation. For example, for the number operator we would write

$$\hat{N}_q = \sum_\mu a_\mu^{q\dagger} a_\mu^q$$

with the commutation relations between single-particle creation and destruction operators described in [1],

$$\left\{ a_\mu^{q'\dagger}, a_\nu^q \right\} = \tau_{\mu\nu}^{qq'} \tag{D.2}$$

$$\left\{ a_\mu^{q'}, a_\nu^q \right\} = \left\{ a_\mu^{q'\dagger}, a_\nu^{q\dagger} \right\} = 0 \tag{D.3}$$

W. Younes et al., *A Microscopic Theory of Fission Dynamics Based on the Generator Coordinate Method*, Lecture Notes in Physics 950,
https://doi.org/10.1007/978-3-030-04424-4

In the special case where $q = q'$, $\tau_{\mu\nu}^{qq'} = \delta_{\mu\nu}$, but in general it is given by the overlap between the single-particle wave functions. In practice, since we consider Hamiltonians that conserve particle number, we will be led to the evaluation of integrals of the form

$$\mathscr{I} = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \, f\left(\varphi' - \varphi\right)$$

where $f(x)$ is a function satisfying the properties

$$f(x + k\pi) = f(x) \tag{D.4}$$

for any integer k, and

$$f^*(x) = f(-x) \tag{D.5}$$

Then by changing variables to

$$\bar{\varphi} = \frac{\varphi + \varphi'}{2}$$
$$\xi = \varphi' - \varphi$$

we reduce the problem to a one-dimensional integral,

$$\mathscr{I} = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\xi \, (2\pi - \xi) \left[f(\xi) + f(-\xi)\right]$$

and by using the properties in Eqs. (D.4) and (D.5), we can reduce this to the result

$$\frac{1}{(2\pi)^2} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \, f\left(\varphi' - \varphi\right) = \frac{1}{\pi} \int_0^{\pi} d\xi \, \mathrm{Re}\left[f(\xi)\right] \tag{D.6}$$

D.2 Norm Overlap

In Eq. (C.38) we wrote a BCS state, adapted for use in particle-number projection integrals, for what follows we will need to write this state with the deformation label q and number of pairs p

$$\begin{aligned}\left|\Phi_q^{(p)}(\varphi)\right\rangle &\equiv \hat{\chi}(\varphi)\left|\Phi_q^{(p)}\right\rangle \\ &= \prod_{\nu>0}\left(u_\nu^q + e^{2i\varphi} v_\nu^q a_\nu^{q\dagger} a_{\bar{\nu}}^{q\dagger}\right)|0\rangle\end{aligned}$$

where $\hat{\chi}(\varphi)$ is the operator defined in Eq. (C.36). We introduce an operator $\hat{X}_q(\varphi)$, analogous to the one in [1], defined by

$$\hat{X}_q(\varphi) \equiv \sum_{\mu>0} e^{2i\varphi} \frac{v_\mu^q}{u_\mu^q} a_\mu^{q\dagger} a_{\bar{\mu}}^{q\dagger}$$
$$\equiv \sum_{\mu>0} e^{2i\varphi} \tan\theta_\mu^q a_\mu^{q\dagger} a_{\bar{\mu}}^{q\dagger}$$

where we have introduced the quantity

$$\tan\theta_\mu^q \equiv \frac{v_\mu^q}{u_\mu^q} \tag{D.7}$$

defined in Eq. (3.21) in [1]. This operator allows us to relate the state $\left|\Phi_q^{(p)}(\varphi)\right\rangle$ to the particle vacuum via

$$\left|\Phi_q^{(p)}(\varphi)\right\rangle = \left\langle 0 \middle| \Phi_q^{(p)}(\varphi)\right\rangle e^{\hat{X}_q(\varphi)} |0\rangle \tag{D.8}$$

and where the normalization is

$$\begin{aligned}\left\langle 0 \middle| \Phi_q^{(p)}(\varphi)\right\rangle &= \left\langle 0 \middle| \prod_{\mu>0} \left(u_\mu^q + e^{2i\varphi} v_\mu^q a_\mu^{q\dagger} a_{\bar{\mu}}^{q\dagger}\right) \middle| 0 \right\rangle \\ &= \prod_{\mu>0} u_\mu^q\end{aligned} \tag{D.9}$$

Then we can generalize Eq. (3.18) in [1] to

$$\begin{aligned}R\left(x,\varphi,\varphi'\right) &= \left\langle 0 \middle| e^{x\hat{X}_q^\dagger(\varphi)} e^{\hat{X}_{q'}(\varphi')} \middle| 0 \right\rangle \\ &\equiv \frac{\left\langle \Phi_q^{(p)}(x,\varphi) \middle| \Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle}{\left\langle \Phi_q^{(p)}(\varphi) \middle| 0 \right\rangle \left\langle 0 \middle| \Phi_{q'}^{(p)}(\varphi')\right\rangle}\end{aligned} \tag{D.10}$$

and the norm overlap is then given by

$$\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle = \left\langle \Phi_q^{(p)}(\varphi) \middle| 0 \right\rangle \left\langle 0 \middle| \Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle R\left(1,\varphi,\varphi'\right) \tag{D.11}$$

We can then differentiate Eq. (D.10) to get

$$\frac{\partial}{\partial x} R\left(x, \varphi, \varphi'\right) = \mathrm{Tr}\left[e^{-2i\varphi} \tan\theta^{q} A\left(x, \varphi, \varphi'\right)\right] \tag{D.12}$$

where $\tan\theta^q$ is a diagonal matrix whose elements are given by Eq. (D.7). The matrix $A\left(x, \varphi, \varphi'\right)$ is defined as

$$A_{\mu\nu}\left(x, \varphi, \varphi'\right) \equiv \frac{\left\langle \Phi_q^{(p)}\left(x, \varphi\right) \left| a_{\bar{\nu}}^{q} a_{\mu}^{q} \right| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle}{\left\langle \Phi_q^{(p)}\left(\varphi\right) \middle| 0 \right\rangle \left\langle 0 \middle| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle} \tag{D.13}$$

We also define a corresponding matrix

$$B_{\mu\nu}\left(x, \varphi, \varphi'\right) \equiv \frac{\left\langle \Phi_q^{(p)}\left(x, \varphi\right) \left| a_{\nu}^{q'\dagger} a_{\bar{\mu}}^{q'\dagger} \right| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle}{\left\langle \Phi_q^{(p)}\left(\varphi\right) \middle| 0 \right\rangle \left\langle 0 \middle| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle} \tag{D.14}$$

Now we can use Eq. (D.8) to write

$$\begin{aligned}
\frac{\left\langle \Phi_q^{(p)}\left(x, \varphi\right) \left| a_{\bar{\nu}}^{q} a_{\mu}^{q} \right| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle}{\left\langle 0 \middle| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle} &= \left\langle \Phi_q^{(p)}\left(x, \varphi\right) \left| a_{\bar{\nu}}^{q} a_{\mu}^{q} e^{\hat{X}_{q'}(\varphi')} \right| 0 \right\rangle \\
&= \left\langle \Phi_q^{(p)}\left(x, \varphi\right) \left| e^{\hat{X}_{q'}(\varphi')} e^{-\hat{X}_{q'}(\varphi')} a_{\bar{\nu}}^{q} a_{\mu}^{q} e^{\hat{X}_{q'}(\varphi')} \right| 0 \right\rangle
\end{aligned}$$

and expand using the Baker-Campbell-Hausdorf relation

$$\begin{aligned}
e^{-\hat{X}_{q'}(\varphi')} a_{\bar{\nu}}^{q} a_{\mu}^{q} e^{\hat{X}_{q'}(\varphi')} &= a_{\bar{\nu}}^{q} a_{\mu}^{q} - \left[\hat{X}_{q'}\left(\varphi'\right), a_{\bar{\nu}}^{q} a_{\mu}^{q}\right] \\
&\quad + \frac{1}{2}\left[\hat{X}_{q'}\left(\varphi'\right), \left[\hat{X}_{q'}\left(\varphi'\right), a_{\bar{\nu}}^{q} a_{\mu}^{q}\right]\right] + \dots
\end{aligned}$$

We can readily show that

$$\left[\hat{X}_{q'}\left(\varphi'\right), a_{\bar{\nu}}^{q} a_{\mu}^{q}\right] = e^{2i\varphi'} \sum_{\alpha>0} \tan\theta_{\alpha}^{q'} \left[\tau_{\bar{\nu}\bar{\alpha}}^{qq'} a_{\alpha}^{q'\dagger} a_{\mu}^{q} + \tau_{\mu\alpha}^{qq'} a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\nu}}^{q} - \tau_{\mu\alpha}^{qq'} \tau_{\bar{\nu}\bar{\alpha}}^{qq'}\right]$$

and

$$\left[\hat{X}_{q'}\left(\varphi'\right), \left[\hat{X}_{q'}\left(\varphi'\right), a_{\bar{\nu}}^{q} a_{\mu}^{q}\right]\right] = -2e^{4i\varphi'} \sum_{\alpha,\beta>0} \tan\theta_{\alpha}^{q'} \tan\theta_{\beta}^{q'} \tau_{\bar{\nu}\bar{\alpha}}^{qq'} \tau_{\mu\beta}^{qq'} a_{\alpha}^{q'\dagger} a_{\bar{\beta}}^{q'\dagger}$$

and clearly, the expansion ends after the second commutator. Therefore we find

$$A_{\mu\nu}\left(x,\varphi,\varphi'\right) = e^{2i\varphi'}\sum_{\alpha>0}\tan\theta_\alpha^{q'}\tau_{\mu\alpha}^{qq'}\tau_{\bar{\nu}\bar{\alpha}}^{qq'}R\left(x,\varphi,\varphi'\right)$$
$$-e^{4i\varphi'}\sum_{\alpha,\beta>0}\tan\theta_\alpha^{q'}\tan\theta_\beta^{q'}\tau_{\bar{\nu}\bar{\alpha}}^{qq'}\tau_{\mu\beta}^{qq'}B_{\beta\alpha}\left(x,\varphi,\varphi'\right)$$

or, in matrix form

$$\boxed{\begin{aligned}A\left(x,\varphi,\varphi'\right) &= e^{2i\varphi'}\tau^{qq'}\tan\theta^{q'}\tau^{qq'\dagger}R\left(x,\varphi,\varphi'\right)\\ &- e^{2i\varphi'}\tau^{qq'}\tan\theta^{q'}B\left(x,\varphi,\varphi'\right)\tau^{qq'}\tan\theta^{q'}\tau^{qq'\dagger}\end{aligned}} \tag{D.15}$$

Next, we need the equation for $B\left(x,\varphi,\varphi'\right)$. Proceeding as for $A\left(x,\varphi,\varphi'\right)$, we calculate

$$\frac{\left\langle\Phi_q^{(p)}\left(x,\varphi\right)\left|a_\nu^{q'\dagger}a_{\bar{\mu}}^{q'\dagger}\right|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle}{\left\langle\Phi_q^{(p)}\left(\varphi\right)\right|0\right\rangle} = \left\langle 0\left|e^{x\hat{X}_q^\dagger(\varphi)}a_\nu^{q'\dagger}a_{\bar{\mu}}^{q'\dagger}e^{-x\hat{X}_q^\dagger(\varphi)}e^{x\hat{X}_q^\dagger(\varphi)}\right|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle$$

We expand again in terms of commutators,

$$e^{x\hat{X}_q^\dagger(\varphi)}a_\nu^{q'\dagger}a_{\bar{\mu}}^{q'\dagger}e^{-x\hat{X}_q^\dagger(\varphi)} = a_\nu^{q'\dagger}a_{\bar{\mu}}^{q'\dagger} + x\left[\hat{X}_q^\dagger\left(\varphi\right), a_\nu^{q'\dagger}a_{\bar{\mu}}^{q'\dagger}\right]$$
$$+\frac{x^2}{2}\left[\hat{X}_q^\dagger\left(\varphi\right),\left[\hat{X}_q^\dagger\left(\varphi\right), a_\nu^{q'\dagger}a_{\bar{\mu}}^{q'\dagger}\right]\right] + \ldots$$

and find

$$\left[\hat{X}_q^\dagger\left(\varphi\right), a_\nu^{q'\dagger}a_{\bar{\mu}}^{q'\dagger}\right] = e^{-2i\varphi}\sum_{\alpha>0}\tan\theta_\alpha^q\left(\tau_{\alpha\nu}^{qq'}\tau_{\bar{\alpha}\bar{\mu}}^{qq'} - \tau_{\bar{\alpha}\bar{\mu}}^{qq'}a_\nu^{q'\dagger}a_\alpha^q - \tau_{\alpha\nu}^{qq'}a_{\bar{\mu}}^{q'\dagger}a_{\bar{\alpha}}^q\right)$$

and

$$\left[\hat{X}_q^\dagger\left(\varphi\right),\left[\hat{X}_q^\dagger\left(\varphi\right), a_\nu^{q'\dagger}a_{\bar{\mu}}^{q'\dagger}\right]\right] = -2e^{-4i\varphi}\sum_{\alpha,\beta>0}\tan\theta_\alpha^q\tan\theta_\beta^q\tau_{\bar{\alpha}\bar{\mu}}^{qq'}\tau_{\beta\nu}^{qq'}a_{\bar{\beta}}^q a_\alpha^q$$

Once again, the expansion ends after the second commutator. Therefore we have

$$B_{\mu\nu}\left(x,\varphi,\varphi'\right) = xe^{-2i\varphi}\sum_{\alpha>0}\tan\theta_\alpha^q\tau_{\alpha\nu}^{qq'}\tau_{\bar{\alpha}\bar{\mu}}^{qq'}R\left(x,\varphi,\varphi'\right)$$
$$-x^2e^{-4i\varphi}\sum_{\alpha,\beta>0}\tan\theta_\alpha^q\tan\theta_\beta^q\tau_{\bar{\alpha}\bar{\mu}}^{qq'}\tau_{\beta\nu}^{qq'}A_{\alpha\beta}\left(x,\varphi,\varphi'\right)$$

which we can write in matrix form

$$\boxed{\begin{aligned} B\left(x,\varphi,\varphi'\right) = {} & xe^{-2i\varphi}\tau^{qq'\dagger}\tan\theta^q\tau^{qq'}R\left(x,\varphi,\varphi'\right) \\ & - x^2e^{-4i\varphi}\tau^{qq'\dagger}\tan\theta^q A\left(x,\varphi,\varphi'\right)\tan\theta^q\tau^{qq'} \end{aligned}} \tag{D.16}$$

To calculate the norm overlap we need to solve Eqs. (D.15) and (D.16) simultaneously, and for this we proceed as in [1] and define

$$C_1\left(x,\varphi,\varphi'\right) \equiv e^{-2i\varphi}\tan\theta^q A\left(x,\varphi,\varphi'\right) \tag{D.17}$$

$$C_2\left(x,\varphi,\varphi'\right) \equiv e^{2i\varphi'}\left(\tau^{qq'\dagger}\right)^{-1}B\left(x,\varphi,\varphi'\right)\tan\theta^{q'}\tau^{qq'\dagger} \tag{D.18}$$

$$M^q\left(\varphi,\varphi'\right) \equiv e^{2i(\varphi'-\varphi)}\tan\theta^q\tau^{qq'}\tan\theta^{q'}\tau^{qq'\dagger} \tag{D.19}$$

Using Eq. (D.15) we can show

$$C_1\left(x,\varphi,\varphi'\right) = M^q\left(\varphi,\varphi'\right)R\left(x,\varphi,\varphi'\right) - M^q\left(\varphi,\varphi'\right)C_2\left(x,\varphi,\varphi'\right) \tag{D.20}$$

and using Eq. (D.16) we get

$$C_2\left(x,\varphi,\varphi'\right) = xM^q\left(\varphi,\varphi'\right)R\left(x,\varphi,\varphi'\right) - x^2C_1\left(x,\varphi,\varphi'\right)M^q\left(\varphi,\varphi'\right) \tag{D.21}$$

Combining Eqs. (D.20) and (D.21) we then find

$$\begin{aligned} C_1\left(x,\varphi,\varphi'\right) = {} & M^q\left(\varphi,\varphi'\right)R\left(x,\varphi,\varphi'\right) - x\left[M^q\left(\varphi,\varphi'\right)\right]^2R\left(x,\varphi,\varphi'\right) \\ & -x^2M^q\left(\varphi,\varphi'\right)C_1\left(x,\varphi,\varphi'\right)M^q\left(\varphi,\varphi'\right) \end{aligned}$$

which we can iterate to find

$$C_1\left(x,\varphi,\varphi'\right) = \left[1 + xM^q\left(\varphi,\varphi'\right)\right]^{-1}M^q\left(\varphi,\varphi'\right)R\left(x,\varphi,\varphi'\right) \tag{D.22}$$

Combining Eqs. (D.12), (D.17), and (D.22) we then get

$$\begin{aligned} \frac{\partial}{\partial x}R\left(x,\varphi,\varphi'\right) &= \mathrm{Tr}\left[e^{-2i\varphi}\tan\theta^q A\left(x,\varphi,\varphi'\right)\right] \\ &= R\left(x,\varphi,\varphi'\right)\mathrm{Tr}\left\{\left[1 + xM^q\left(\varphi,\varphi'\right)\right]^{-1}M^q\left(\varphi,\varphi'\right)\right\} \end{aligned}$$

Next, we integrate this result from $x = 0$ to $x = 1$

$$\ln\frac{R\left(1,\varphi,\varphi'\right)}{R\left(0,\varphi,\varphi'\right)} = \int_0^1 dx\,\frac{\partial}{\partial x}\mathrm{Tr}\left\{\ln\left[1 + xM^q\left(\varphi,\varphi'\right)\right]\right\}$$

By inspection of Eq. (D.10) we can see that $R\left(0, \varphi, \varphi'\right) = 1$, and therefore

$$R\left(1, \varphi, \varphi'\right) = \exp\left\{\mathrm{Tr}\left\{\ln\left[1 + M^q\left(\varphi, \varphi'\right)\right]\right\}\right\}$$

By a corollary to Jacobi's formula for the derivative of a matrix determinant, this can be written as

$$R\left(1, \varphi, \varphi'\right) = \det\left[1 + M^q\left(\varphi, \varphi'\right)\right] \tag{D.23}$$

Using this result in Eq. (D.11), and with the normalization given by Eq. (D.9) we get

$$\left\langle \Phi_q^{(p)}\left(\varphi\right) \middle| \Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle = \left(\prod_{\mu>0} u_\mu^q u_\mu^{q'}\right) \det\left[1 + e^{2i\left(\varphi'-\varphi\right)} M^q\right] \tag{D.24}$$

where we have explicitly factored out the dependence on $\varphi' - \varphi$ by writing

$$M^q\left(\varphi, \varphi'\right) = e^{2i\left(\varphi'-\varphi\right)} M^q$$

with M^q defined as in Eq. (3.33) of [1],

$$M^q \equiv \tan\theta^q \tau^{qq'} \tan\theta^{q'} \tau^{qq'\dagger}$$

All that remains now is to integrate Eq. (D.24) to obtain the projected norm overlap as in Eq. (D.1),

$$\left\langle \Phi_q^{(p)} \middle| P_q^{(N)\dagger} P_{q'}^{(N)} \middle| \Phi_{q'}^{(p)}\right\rangle = \frac{1}{(2\pi)^2}\int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \, f\left(\varphi' - \varphi\right)$$

where the function

$$f\left(\varphi' - \varphi\right) \equiv e^{-i\left(\varphi'-\varphi\right)N}\left(\prod_{\mu>0} u_\mu^q u_\mu^{q'}\right)\det\left[1 + e^{2i\left(\varphi'-\varphi\right)} M^q\right]$$

clearly satisfies Eqs. (D.4) and (D.5) for and even number $N = 2p$ of particles. Therefore, we can use Eq. (D.6) to reduce the integral to

$$\begin{aligned}\left\langle \Phi_q^{(p)} \middle| P_q^{(N)\dagger} P_{q'}^{(N)} \middle| \Phi_{q'}^{(p)}\right\rangle = \frac{1}{\pi}\left(\prod_{\mu>0} u_\mu^q u_\mu^{q'}\right)\int_0^{\pi} d\xi \\ \times \mathrm{Re}\left\{e^{-i\xi N}\det\left[1 + e^{2i\xi} M^q\right]\right\}\end{aligned} \tag{D.25}$$

We now assume that M^q can be diagonalized,

$$\boxed{M^q = S D^q S^T} \tag{D.26}$$

where S is an orthogonal matrix and D^q is a diagonal matrix. Then,

$$\det\left[1 + e^{2i\xi} M^q\right] = \prod_{\mu>0} \left(1 + e^{2i\xi} D^q_{\mu\mu}\right) \tag{D.27}$$

It will be convenient to write the complex number $1 + e^{2i\xi} D^q_{\mu\mu}$ in exponential form,

$$1 + e^{2i\xi} D^q_{\mu\mu} = n_\mu (\xi)\, e^{i\Omega_\mu(\xi)}$$

where

$$\boxed{n_\mu (\xi) = \sqrt{1 + 2\cos(2\xi)\, D_{\mu\mu} + D^2_{\mu\mu}}} \tag{D.28}$$

and[1]

$$\boxed{\Omega_\mu (\xi) = \tan^{-1}\left(1 + \cos(2\xi)\, D_{\mu\mu}, \sin(2\xi)\, D_{\mu\mu}\right)} \tag{D.29}$$

Using these results, we can write the determinant in Eq. (D.27) as

$$\det\left[1 + e^{2i\xi} M^q\right] = n(\xi)\, e^{i\Omega(\xi)}$$

where we have defined

$$\boxed{n(\xi) \equiv \prod_{\mu>0} n_\mu (\xi)} \tag{D.30}$$

and

$$\boxed{\Omega(\xi) \equiv \sum_{\mu>0} \Omega_\mu (\xi)} \tag{D.31}$$

Thus we have

$$\left\langle \Phi^{(p)}_q (\varphi) \middle| \Phi^{(p)}_{q'} (\varphi') \right\rangle = \left(\prod_{\mu>0} u^q_\mu u^{q'}_\mu \right) n(\xi)\, e^{i\Omega(\xi)} \tag{D.32}$$

[1]We use the two-argument arctangent function, $\tan^{-1}(x, y)$, which is defined as $\mathrm{atan2}(y, x)$ in some computer languages.

Returning to the overlap integral in Eq. (D.25), we now have

$$\boxed{\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi} \left(\prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) \int_0^\pi d\xi \, n\left(\xi\right) \cos\left[\Omega\left(\xi\right) - N\xi\right]} \tag{D.33}$$

and the remaining integral can be evaluated numerically, as discussed in Sect. C.4.

D.3 Generalized One-Body Density

D.3.1 Preliminary Definitions and Results

We introduce the matrix

$$M^{q'}\left(\varphi, \varphi'\right) \equiv e^{2i\varphi'} \tan\theta^{q'} \tau^{qq'\dagger} e^{-2i\varphi} \tan\theta^q \tau^{qq'} \tag{D.34}$$

which is related to the matrix $M^{q'}$ defined in Eq. (3.44) of [1] via

$$M^{q'}\left(\varphi, \varphi'\right) = e^{2i\left(\varphi'-\varphi\right)} M^{q'}$$

Note that using Eq. (D.19), we have

$$e^{2i\varphi'} \tan\theta^{q'} \tau^{qq'\dagger} M^q\left(\varphi, \varphi'\right) = M^{q'}\left(\varphi, \varphi'\right) e^{2i\varphi'} \tan\theta^{q'} \tau^{qq'\dagger}$$

and

$$M^q\left(\varphi, \varphi'\right) e^{-2i\varphi} \tan\theta^q \tau^{qq'} = e^{-2i\varphi} \tan\theta^q \tau^{qq'} M^{q'}\left(\varphi, \varphi'\right)$$

from this, we deduce

$$e^{2i\varphi'} \tan\theta^{q'} \tau^{qq'\dagger} M^q\left(\varphi, \varphi'\right) e^{-2i\varphi} \tan\theta^q \tau^{qq'} = \left[M^{q'}\left(\varphi, \varphi'\right)\right]^2$$

More generally, we can show by induction that for any non-negative integer n,

$$\boxed{e^{2i\varphi'} \tan\theta^{q'} \tau^{qq'\dagger} \left[M^q\left(\varphi, \varphi'\right)\right]^n e^{-2i\varphi} \tan\theta^q \tau^{qq'} = \left[M^{q'}\left(\varphi, \varphi'\right)\right]^{n+1}} \tag{D.35}$$

We now derive some useful equations for the matrices $A\left(x, \varphi, \varphi'\right)$ and $B\left(x, \varphi, \varphi'\right)$ defined in Eqs. (D.13) and (D.14), respectively. First, by combining Eqs. (D.17) and (D.22), we get

$$e^{-2i\varphi}\tan\theta^{q}A\left(x,\varphi,\varphi'\right)=\left[1+xM^{q}\left(\varphi,\varphi'\right)\right]^{-1}M^{q}\left(\varphi,\varphi'\right)R\left(x,\varphi,\varphi'\right) \tag{D.36}$$

Then from Eq. (D.16), we get

$$\begin{aligned}e^{2i\varphi'}\tan\theta^{q'}B\left(x,\varphi,\varphi'\right)&=xR\left(x,\varphi,\varphi'\right)e^{2i\varphi'}\tan\theta^{q'}\tau^{qq'\dagger}\{1-\\&\qquad-\left[1+xM^{q}\left(\varphi,\varphi'\right)\right]^{-1}xM^{q}\left(\varphi,\varphi'\right)\Big\}\,e^{-2i\varphi}\tan\theta^{q}\tau^{qq'}\\&=xR\left(x,\varphi,\varphi'\right)e^{2i\varphi'}\tan\theta^{q'}\tau^{qq'\dagger}\left[1+xM^{q}\left(\varphi,\varphi'\right)\right]^{-1}\\&\qquad\times e^{-2i\varphi}\tan\theta^{q}\tau^{qq'}\end{aligned}$$

Now we can use Eq. (D.35) to obtain the equivalent to Eq. (3.43) in [1],

$$\boxed{e^{2i\varphi'}\tan\theta^{q'}B\left(x,\varphi,\varphi'\right)=xR\left(x,\varphi,\varphi'\right)\left[1+xM^{q'}\left(\varphi,\varphi'\right)\right]^{-1}M^{q'}\left(\varphi,\varphi'\right)} \tag{D.37}$$

We can also get an equation for $B\left(x,\varphi,\varphi'\right)$ alone by using Eq. (D.36) in Eq. (D.16), then

$$\begin{aligned}B\left(x,\varphi,\varphi'\right)&=xR\left(x,\varphi,\varphi'\right)\tau^{qq'\dagger}\left\{I-x\left[1+xM^{q}\left(\varphi,\varphi'\right)\right]^{-1}M^{q}\left(\varphi,\varphi'\right)\right\}\\&\qquad\times e^{-2i\varphi}\tan\theta^{q}\tau^{qq'}\\&=xR\left(x,\varphi,\varphi'\right)\tau^{qq'\dagger}\left[1+xM^{q}\left(\varphi,\varphi'\right)\right]^{-1}e^{-2i\varphi}\tan\theta^{q}\tau^{qq'}\end{aligned}$$

We will need in particular the equation for $B\left(1,\varphi,\varphi'\right)$ which we get from this last equation,

$$\boxed{B\left(1,\varphi,\varphi'\right)=R\left(1,\varphi,\varphi'\right)\tau^{qq'\dagger}\left[1+M^{q}\left(\varphi,\varphi'\right)\right]^{-1}e^{-2i\varphi}\tan\theta^{q}\tau^{qq'}} \tag{D.38}$$

This is the equivalent to Eq. (3.45) in [1]

D.3.2 Projected Matrix Elements of $a^{\dagger}a$

We now consider

$$\left\langle\Phi_{q}^{(p)}\left|P_{q}^{(N)\dagger}a_{\alpha}^{q'\dagger}a_{\beta}^{q'}P_{q'}^{(N)}\right|\Phi_{q'}^{(p)}\right\rangle=\frac{1}{(2\pi)^{2}}\int_{0}^{2\pi}d\varphi\int_{0}^{2\pi}d\varphi'\,e^{-i(\varphi'-\varphi)N}\times\left\langle\Phi_{q}^{(p)}\left|e^{-i\hat{N}_{q}\varphi}a_{\alpha}^{q'\dagger}a_{\beta}^{q'}e^{i\hat{N}_{q'}\varphi'}\right|\Phi_{q'}^{(p)}\right\rangle \tag{D.39}$$

where we will assume for now $\alpha, \beta > 0$. We focus on the matrix element in the integrand,

$$\left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle = \left\langle \Phi_q^{(p)} (\varphi) \left| a_\alpha^{q'\dagger} a_\beta^{q'} \right| \Phi_{q'}^{(p)} (\varphi') \right\rangle$$

Then we use Eq. (D.8) to write

$$\begin{aligned} &\left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle \\ &= \left\langle 0 | \, \Phi_{q'}^{(p)} (\varphi') \right\rangle \left\langle \Phi_q^{(p)} (\varphi) \left| e^{\hat{X}_{q'}(\varphi')} e^{-\hat{X}_{q'}(\varphi')} a_\alpha^{q'\dagger} a_\beta^{q'} e^{\hat{X}_{q'}(\varphi')} \right| 0 \right\rangle \end{aligned}$$

Then we proceed as in appendix 3 of [1] and expand

$$\begin{aligned} e^{-\hat{X}_{q'}(\varphi')} a_\alpha^{q'\dagger} a_\beta^{q'} e^{\hat{X}_{q'}(\varphi')} = a_\alpha^{q'\dagger} a_\beta^{q'} &- \left[\hat{X}_{q'} (\varphi') , a_\alpha^{q'\dagger} a_\beta^{q'} \right] \\ &+ \frac{1}{2} \left[\hat{X}_{q'} (\varphi') , \left[\hat{X}_{q'} (\varphi') , a_\alpha^{q'\dagger} a_\beta^{q'} \right] \right] + \dots \end{aligned}$$

The first commutator is

$$\left[\hat{X}_{q'} (\varphi') , a_\alpha^{q'\dagger} a_\beta^{q'} \right] = -e^{2i\varphi'} \tan\theta_\beta^{q'} a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger}$$

and the higher-order commutators therefore vanish. Thus we can write

$$\begin{aligned} \left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle &= \left\langle 0 | \, \Phi_{q'}^{(p)} (\varphi') \right\rangle e^{2i\varphi'} \tan\theta_\beta^{q'} \\ &\quad \times \left\langle \Phi_q^{(p)} (\varphi) \left| e^{\hat{X}_{q'}(\varphi')} a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger} \right| 0 \right\rangle \\ &= e^{2i\varphi'} \tan\theta_\beta^{q'} \left\langle \Phi_q^{(p)} (\varphi) \left| a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger} \right| \Phi_{q'}^{(p)} (\varphi') \right\rangle \end{aligned}$$

Now going back to the definition of B in Eq. (D.14), we can write this as

$$\begin{aligned} \left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle &= e^{2i\varphi'} \tan\theta_\beta^{q'} \left\langle \Phi_q^{(p)} (\varphi) \middle| 0 \right\rangle \left\langle 0 | \, \Phi_{q'}^{(p)} (\varphi') \right\rangle \\ &\quad \times B_{\beta\alpha} (1, \varphi, \varphi') \end{aligned} \tag{D.40}$$

Using Eq. (D.37) with $x = 1$ we can write this as

$$\begin{aligned} \left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle &= \left\langle \Phi_q^{(p)} (\varphi) \middle| 0 \right\rangle \left\langle 0 | \, \Phi_{q'}^{(p)} (\varphi') \right\rangle \\ &\quad \times R (1, \varphi, \varphi') \left\{ \left[1 + M^{q'} (\varphi, \varphi') \right]^{-1} M^{q'} (\varphi, \varphi') \right\}_{\beta\alpha} \end{aligned}$$

Next, we use Eq. (D.11) to write this as

$$\left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle = \left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle \times \left\{ \left[1 + M^{q'}(\varphi, \varphi') \right]^{-1} M^{q'}(\varphi, \varphi') \right\}_{\beta\alpha} \tag{D.41}$$

We already obtained an explicit form for the overlap $\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle$ in Eq. (D.32),

$$\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle = \left(\prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) n(\xi)\, e^{i\Omega(\xi)}$$

For the remaining term in Eq. (D.41), we assume that $M^{q'}$ can be diagonalized,

$$M^{q'} = S' D^{q'} S'^T \tag{D.42}$$

where S' is an orthogonal matrix and $D^{q'}$ is a diagonal matrix. Then,

$$\left[1 + M^{q'}(\varphi, \varphi') \right]^{-1} M^{q'}(\varphi, \varphi') = S' \left(1 + e^{2i\xi} D^{q'} \right)^{-1} e^{2i\xi} D^{q'} S'^T$$

where we have used $\xi \equiv \varphi' - \varphi$. The matrix $\left(1 + e^{2i\xi} D^{q'} \right)^{-1} e^{2i\xi} D^{q'}$ is diagonal, and its elements are

$$\left[\left(1 + e^{2i\xi} D^{q'} \right)^{-1} e^{2i\xi} D^{q'} \right]_{\mu\mu} = e^{2i\xi} \frac{D_{\mu\mu}^{q'} \left[1 + D_{\mu\mu}^{q'} \cos(2\xi) - i \sin(2\xi) \right]}{1 + 2D_{\mu\mu}^{q'} \cos(2\xi) + \left(D_{\mu\mu}^{q'} \right)^2}$$

From this we calculate

$$\left\{ \left[1 + M^{q'}(\varphi, \varphi') \right]^{-1} M^{q'}(\varphi, \varphi') \right\}_{\beta\alpha} = e^{2i\xi} \sum_{\mu>0} S'_{\beta\mu} S'_{\alpha\mu} \frac{D_{\mu\mu}^{q'} \left[1 + D_{\mu\mu}^{q'} \cos(2\xi) - i D_{\mu\mu}^{q'} \sin(2\xi) \right]}{1 + 2D_{\mu\mu}^{q'} \cos(2\xi) + \left(D_{\mu\mu}^{q'} \right)^2}$$

Separating out the real and imaginary parts from the quantity in the summation,

$$W'_{\beta\alpha}(\xi) \equiv \sum_{\mu>0} S'_{\beta\mu} S'_{\alpha\mu} \frac{D^{q'}_{\mu\mu}\left[1 + D^{q'}_{\mu\mu}\cos(2\xi)\right]}{1 + 2D^{q'}_{\mu\mu}\cos(2\xi) + \left(D^{q'}_{\mu\mu}\right)^2} \tag{D.43}$$

$$Z'_{\beta\alpha}(\xi) \equiv -\sum_{\mu>0} S'_{\beta\mu} S'_{\alpha\mu} \frac{\left(D^{q'}_{\mu\mu}\right)^2 \sin(2\xi)}{1 + 2D^{q'}_{\mu\mu}\cos(2\xi) + \left(D^{q'}_{\mu\mu}\right)^2} \tag{D.44}$$

we can write the matrix element in exponential form

$$\begin{aligned} \left\{\left[1 + M^{q'}\left(\varphi, \varphi'\right)\right]^{-1} M^{q'}\left(\varphi, \varphi'\right)\right\}_{\beta\alpha} &= e^{2i\xi}\left[W'_{\beta\alpha}(\xi) + iZ'_{\beta\alpha}(\xi)\right] \\ &\equiv n'_{\beta\alpha}(\xi)\, e^{i\left[\Omega'_{\beta\alpha}(\xi)+2\xi\right]} \end{aligned} \tag{D.45}$$

where

$$\begin{aligned} n'_{\beta\alpha}(\xi) &= \sqrt{\left[W'_{\beta\alpha}(\xi)\right]^2 + \left[Z'_{\beta\alpha}(\xi)\right]^2} \\ \Omega'_{\beta\alpha}(\xi) &= \tan^{-1}\left(W'_{\beta\alpha}(\xi), Z'_{\beta\alpha}(\xi)\right) \end{aligned}$$

The matrix element in Eq. (D.41) can then be written as

$$\begin{aligned} \left\langle \Phi^{(p)}_q \left| e^{-i\hat{N}_q\varphi} a^{q'\dagger}_\alpha a^{q'}_\beta e^{i\hat{N}_{q'}\varphi'} \right| \Phi^{(p)}_{q'} \right\rangle = \left(\prod_{\mu>0} u^q_\mu u^{q'}_\mu\right) n(\xi)\, e^{i\Omega(\xi)} n'_{\beta\alpha}(\xi) \\ \times\, e^{i\left[\Omega'_{\beta\alpha}(\xi)+2\xi\right]} \end{aligned} \tag{D.46}$$

We can also define the following quantity which will be useful in Sect. D.4,

$$\begin{aligned} S_{\beta\alpha}\left(\varphi, \varphi'\right) &\equiv \frac{\left\langle \Phi^{(p)}_q(\varphi) \left| a^{q'\dagger}_\alpha a^{q'}_\beta \right| \Phi^{(p)}_{q'}\left(\varphi'\right)\right\rangle}{\left\langle \Phi^{(p)}_q(\varphi) \middle| \Phi^{(p)}_{q'}\left(\varphi'\right)\right\rangle} \\ &= e^{2i\xi}\left[W'_{\beta\alpha}(\xi) + iZ'_{\beta\alpha}(\xi)\right] \end{aligned} \tag{D.47}$$

We can now return to Eq. (D.39) and define the function

$$f\left(\varphi' - \varphi\right) \equiv e^{-i\left(\varphi'-\varphi\right)N} \left(\prod_{\mu>0} u^q_\mu u^{q'}_\mu\right) \det\left[1 + e^{2i\left(\varphi'-\varphi\right)} M^q\right]$$

$$\times \left\{ \left[1 + e^{2i(\varphi'-\varphi)} M^{q'} \right]^{-1} e^{2i(\varphi'-\varphi)} M^{q'} \right\}_{\beta\alpha}$$

which clearly satisfies Eqs. (D.4) and (D.5) for and even number $N = 2p$ of particles. Therefore, we can use Eq. (D.6) to reduce the integral in Eq. (D.39) to one dimension, and use the exponential forms derived above to simplify Eq. (D.41). The result is

$$\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} a_\alpha^{q'\dagger} a_\beta^{q'} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi} \left(\prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) \int_0^\pi d\xi \, \mathrm{Re} \left[e^{-i\xi N} n(\xi) \, e^{i\Omega(\xi)} n'_{\beta\alpha}(\xi) \, e^{i\left[\Omega'_{\beta\alpha}(\xi)+2\xi\right]} \right]$$

or

$$\boxed{\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} a_\alpha^{q'\dagger} a_\beta^{q'} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi} \left(\prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) \int_0^\pi d\xi \, n(\xi) \, n'_{\beta\alpha}(\xi) \times \cos\left[\Omega(\xi) + \Omega'_{\beta\alpha}(\xi) - \xi(N-2) \right]} \tag{D.48}$$

We can proceed along similar lines to derive the projected one-body overlap for the time-reversed states, $\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle$. We note that

$$\left[\hat{X}_{q'}(\varphi'), a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'} \right] = -e^{2i\varphi'} \tan\theta_\beta^{q'} a_\beta^{q'\dagger} a_{\bar{\alpha}}^{q'\dagger}$$

and therefore Eq. (D.40) becomes

$$\begin{aligned} \left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle &= e^{2i\varphi'} \tan\theta_\beta^{q'} \left\langle \Phi_q^{(p)}(\varphi) \middle| 0 \right\rangle \left\langle 0 \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle \\ &\quad \times B_{\alpha\beta}(1, \varphi, \varphi') \\ &= \left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle \\ &\quad \times \frac{B_{\alpha\beta}(1, \varphi, \varphi')}{R(1, \varphi, \varphi')} e^{2i\varphi'} \tan\theta_\beta^{q'} \end{aligned} \tag{D.49}$$

Next, we examine the effect on this result of simultaneously exchanging $\alpha \leftrightarrow \beta$, $\varphi \leftrightarrow \varphi'$, and $q \leftrightarrow q'$. We denote the operation which consists in making those exchanges by the superscript symbol $\leftrightarrow$. Clearly,

$$\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle = \left[\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle^{\leftrightarrow} \right]^*$$

and from Eq. (D.10),

$$R\left(1,\varphi,\varphi'\right)=\left[\left[R\left(1,\varphi,\varphi'\right)\right]^{\leftrightarrow}\right]^{*}$$

Then, from Eqs. (D.13) and (D.14),

$$B_{\alpha\beta}\left(1,\varphi,\varphi'\right)=\left[\left[A_{\alpha\beta}\left(1,\varphi,\varphi'\right)\right]^{\leftrightarrow}\right]^{*}$$

And we can also write

$$e^{2i\varphi'}\tan\theta_{\beta}^{q'}=\left[\left(e^{-2i\varphi}\tan\theta_{\alpha}^{q}\right)^{\leftrightarrow}\right]^{*}$$

Thus Eq. (D.49) becomes

$$\left\langle \Phi_q^{(p)}\left|e^{-i\hat{N}_q\varphi}a_{\bar{\alpha}}^{q'\dagger}a_{\bar{\beta}}^{q'}e^{i\hat{N}_{q'}\varphi'}\right|\Phi_{q'}^{(p)}\right\rangle=\left\{\left[\left\langle \Phi_q^{(p)}\left(\varphi\right)\middle|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle\right.\right.$$
$$\left.\left.\times e^{-2i\varphi}\tan\theta_{\alpha}^{q}\frac{A_{\alpha\beta}\left(1,\varphi,\varphi'\right)}{R\left(1,\varphi,\varphi'\right)}\right]^{\leftrightarrow}\right\}^{*}$$

and using Eq. (D.36) with $x=1$, this simplifies to

$$\left\langle \Phi_q^{(p)}\left|e^{-i\hat{N}_q\varphi}a_{\bar{\alpha}}^{q'\dagger}a_{\bar{\beta}}^{q'}e^{i\hat{N}_{q'}\varphi'}\right|\Phi_{q'}^{(p)}\right\rangle=\left\{\left[\left\langle \Phi_q^{(p)}\left(\varphi\right)\middle|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle\right.\right.$$
$$\left.\left.\times\left[\left[1+M^{q}\left(\varphi,\varphi'\right)\right]^{-1}M^{q}\left(\varphi,\varphi'\right)\right]_{\alpha\beta}\right]^{\leftrightarrow}\right\}^{*}$$
$$=\left\langle \Phi_q^{(p)}\left(\varphi\right)\middle|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle$$
$$\times\left[\left[1+M^{q'}\left(\varphi,\varphi'\right)\right]^{-1}M^{q'}\left(\varphi,\varphi'\right)\right]_{\beta\alpha}$$

where we have used Eq. (D.34) to write

$$\left[M^{q'}\left(\varphi',\varphi\right)\right]^{*}=M^{q'}\left(\varphi,\varphi'\right)$$

Comparing with Eq. (D.41) it is clear that

$$\left\langle \Phi_q^{(p)}\left|e^{-i\hat{N}_q\varphi}a_{\bar{\alpha}}^{q'\dagger}a_{\bar{\beta}}^{q'}e^{i\hat{N}_{q'}\varphi'}\right|\Phi_{q'}^{(p)}\right\rangle=\left\langle \Phi_q^{(p)}\left|e^{-i\hat{N}_q\varphi}a_{\alpha}^{q'\dagger}a_{\beta}^{q'}e^{i\hat{N}_{q'}\varphi'}\right|\Phi_{q'}^{(p)}\right\rangle \tag{D.50}$$

and therefore

$$\boxed{\left\langle \Phi_q^{(p)}\left|e^{-i\hat{N}_q\varphi}a_{\bar{\alpha}}^{q'\dagger}a_{\bar{\beta}}^{q'}e^{i\hat{N}_{q'}\varphi'}\right|\Phi_{q'}^{(p)}\right\rangle=\left\langle \Phi_q^{(p)}\left|P_q^{(N)\dagger}a_{\alpha}^{q'\dagger}a_{\beta}^{q'}P_{q'}^{(N)}\right|\Phi_{q'}^{(p)}\right\rangle} \tag{D.51}$$

D.3.3 Calculation of the Matrix Elements $\left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'} a_{\bar\beta}^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle$

As usual, we write

$$\left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'} a_{\bar\beta}^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = \left\langle \Phi_q^{(p)}(\varphi) \left| e^{\hat X_{q'}(\varphi')} e^{-\hat X_{q'}(\varphi')} a_\alpha^{q'} a_{\bar\beta}^{q'} e^{\hat X_{q'}(\varphi')} \right| 0 \right\rangle$$

and expand

$$e^{-\hat X_{q'}(\varphi')} a_\alpha^{q'} a_{\bar\beta}^{q'} e^{\hat X_{q'}(\varphi')} = a_\alpha^{q'} a_{\bar\beta}^{q'} - \left[\hat X_{q'}(\varphi'), a_\alpha^{q'} a_{\bar\beta}^{q'} \right] + \frac{1}{2} \left[\hat X_{q'}(\varphi'), \left[\hat X_{q'}(\varphi'), a_\alpha^{q'} a_{\bar\beta}^{q'} \right] \right] + \ldots$$

The first commutator is

$$\left[\hat X_{q'}(\varphi'), a_\alpha^{q'} a_{\bar\beta}^{q'} \right] = e^{2i\varphi'} \left[\delta_{\alpha\beta} \tan\theta_\beta^{q'} - \tan\theta_\alpha^{q'} a_{\bar\alpha}^{q'\dagger} a_{\bar\beta}^{q'} - \tan\theta_\beta^{q'} a_\beta^{q'\dagger} a_\alpha^{q'} \right]$$

and the second is

$$\left[\hat X_{q'}(\varphi'), \left[\hat X_{q'}(\varphi'), a_\alpha^{q'} a_{\bar\beta}^{q'} \right] \right] = 2e^{4i\varphi'} \tan\theta_\alpha^{q'} \tan\theta_\beta^{q'} a_\beta^{q'\dagger} a_{\bar\alpha}^{q'\dagger}$$

and the expansion therefore stops at the second commutator. Thus we have

$$\begin{aligned} \left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'} a_{\bar\beta}^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = & -\delta_{\alpha\beta} e^{2i\varphi'} \tan\theta_\beta^{q'} \left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle \\ & + e^{2i\varphi'} \tan\theta_\alpha^{q'} e^{2i\varphi'} \tan\theta_\beta^{q'} \\ & \times \left\langle \Phi_q^{(p)}(\varphi) \left| a_\beta^{q'\dagger} a_{\bar\alpha}^{q'\dagger} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle \end{aligned}$$

Now, from Eqs. (D.14) and (D.10) we can write

$$\left\langle \Phi_q^{(p)}(\varphi) \left| a_\beta^{q'\dagger} a_{\bar\alpha}^{q'\dagger} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = \frac{\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle}{R(1, \varphi, \varphi')} B_{\alpha\beta}(1, \varphi, \varphi')$$

and using Eq. (D.37), we finally obtain

$$\begin{aligned} \left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'} a_{\bar\beta}^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = & -\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle \\ & \times \left\{ \left[1 + M^{q'}(\varphi, \varphi') \right]^{-1} e^{2i\varphi'} \tan\theta^{q'} \right\}_{\alpha\beta} \end{aligned} \tag{D.52}$$

which is the equivalent to Eq. (3.47) in [1]. The explicit expression for $\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle$ is given by Eq. (D.32). For the remaining term, we proceed as in Sect. D.3.2 and use the diagonalized form of $M^{q'}$ in Eq. (D.42) to write

$$\left\{ \left[1 + M^{q'}(\varphi, \varphi') \right]^{-1} e^{2i\varphi'} \tan\theta^{q'} \right\}_{\alpha\beta} = e^{2i\varphi'} \sum_{\mu>0} S'_{\beta\mu} S'_{\alpha\mu} \frac{\tan\theta_\mu^{q'} \left[1 + D_{\mu\mu}^{q'} \cos(2\xi) - i D_{\mu\mu}^{q'} \sin(2\xi) \right]}{1 + 2D_{\mu\mu}^{q'} \cos(2\xi) + \left(D_{\mu\mu}^{q'} \right)^2}$$

where we have set $\xi = \varphi' - \varphi$. We can then define

$$W_{\beta\alpha}^{(-)}(\xi) \equiv \sum_{\mu>0} S'_{\beta\mu} S'_{\alpha\mu} \frac{\tan\theta_\mu^{q'} \left[1 + D_{\mu\mu}^{q'} \cos(2\xi) \right]}{1 + 2D_{\mu\mu}^{q'} \cos(2\xi) + \left(D_{\mu\mu}^{q'} \right)^2} \tag{D.53}$$

$$Z_{\beta\alpha}^{(-)}(\xi) \equiv -\sum_{\mu>0} S'_{\beta\mu} S'_{\alpha\mu} \frac{\tan\theta_\mu^{q'} D_{\mu\mu}^{q'} \sin(2\xi)}{1 + 2D_{\mu\mu}^{q'} \cos(2\xi) + \left(D_{\mu\mu}^{q'} \right)^2} \tag{D.54}$$

and write the matrix element in exponential form

$$\begin{aligned} \left\{ \left[1 + M^{q'}(\varphi, \varphi') \right]^{-1} e^{2i\varphi'} \tan\theta^{q'} \right\}_{\alpha\beta} &= e^{2i\varphi'} \left[W_{\beta\alpha}^{(-)}(\xi) + i Z_{\beta\alpha}^{(-)}(\xi) \right] \\ &\equiv e^{2i\varphi'} n_{\beta\alpha}^{(-)}(\xi) \, e^{i\Omega_{\beta\alpha}^{(-)}(\xi)} \end{aligned}$$

where

$$n_{\beta\alpha}^{(-)}(\xi) = \sqrt{\left[W_{\beta\alpha}^{(-)}(\xi) \right]^2 + \left[Z_{\beta\alpha}^{(-)}(\xi) \right]^2}$$

$$\Omega_{\beta\alpha}^{(-)}(\xi) = \tan^{-1}\left(W_{\beta\alpha}^{(-)}(\xi), Z_{\beta\alpha}^{(-)}(\xi) \right)$$

Putting all these results together, we find

$$\begin{aligned} \left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'} a_{\bar\beta}^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = -e^{2i\varphi'} \left(\prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) n(\xi) \, e^{i\Omega(\xi)} \\ \times n_{\beta\alpha}^{(-)}(\xi) \, e^{i\Omega_{\beta\alpha}^{(-)}(\xi)} \end{aligned} \tag{D.55}$$

Note that, because of the fact that the operator $a^{q'}_{\alpha} a^{q'}_{\bar{\beta}}$ does not conserve particle number, this matrix element does not depend on ξ alone, but on φ' as well. However, this matrix element will usually be combined with $\left\langle \Phi^{(p)}_q \middle| P^{(N)\dagger}_q a^{q'\dagger}_{\alpha} a^{q'\dagger}_{\bar{\beta}} P^{(N)}_{q'} \middle| \Phi^{(p)}_{q'} \right\rangle$ in calculations of the interaction matrix elements, and the product will again depend on ξ alone, as we will see in Sect. D.3.4. We also define at this point the quantity

$$
\begin{aligned}
Y_{\alpha\bar{\beta}}\left(\varphi, \varphi'\right) &\equiv \frac{\left\langle \Phi^{(p)}_q (\varphi) \middle| a^{q'}_{\alpha} a^{q'}_{\bar{\beta}} \middle| \Phi^{(p)}_{q'} \left(\varphi'\right) \right\rangle}{\left\langle \Phi^{(p)}_q (\varphi) \middle| \Phi^{(p)}_{q'} (\varphi') \right\rangle} \\
&= -e^{2i\varphi'} \left[W^{(-)}_{\beta\alpha} (\xi) + i Z^{(-)}_{\beta\alpha} (\xi) \right]
\end{aligned}
\tag{D.56}
$$

which will be useful in Sect. D.4.

D.3.4 Calculation of the Matrix Elements $\left\langle \Phi^{(p)}_q \middle| P^{(N)\dagger}_q a^{q'\dagger}_{\alpha} a^{q'\dagger}_{\bar{\beta}} P^{(N)}_{q'} \middle| \Phi^{(p)}_{q'} \right\rangle$

Using Eq. (D.14) we write

$$
\left\langle \Phi^{(p)}_q (\varphi) \middle| a^{q'\dagger}_{\alpha} a^{q'\dagger}_{\bar{\beta}} \middle| \Phi^{(p)}_{q'} \left(\varphi'\right) \right\rangle = \left\langle \Phi^{(p)}_q (\varphi) \middle| 0 \right\rangle \left\langle 0 \middle| \Phi^{(p)}_{q'} \left(\varphi'\right) \right\rangle B_{\beta\alpha} \left(x, \varphi, \varphi'\right)
$$

Using Eqs. (D.11) and (D.38) (with $x = 1$) this becomes

$$
\begin{aligned}
\left\langle \Phi^{(p)}_q (\varphi) \middle| a^{q'\dagger}_{\alpha} a^{q'\dagger}_{\bar{\beta}} \middle| \Phi^{(p)}_{q'} \left(\varphi'\right) \right\rangle &= \left\langle \Phi^{(p)}_q (\varphi) \middle| \Phi^{(p)}_{q'} \left(\varphi'\right) \right\rangle \\
&\times \left[\tau^{qq'\dagger} \left[1 + M^q \left(\varphi, \varphi'\right)\right]^{-1} e^{-2i\varphi} \tan\theta^q \tau^{qq'} \right]_{\beta\alpha}
\end{aligned}
\tag{D.57}
$$

which is the equivalent to Eq. (3.48) in [1]. The explicit expression for $\left\langle \Phi^{(p)}_q (\varphi) \middle| \Phi^{(p)}_{q'} \left(\varphi'\right) \right\rangle$ is given by Eq. (D.32). For the remaining term we can use the diagonalized form of M^q in Eq. (D.26) and write

$$
\begin{aligned}
&\left[\tau^{qq'\dagger} \left[1 + M^q \left(\varphi, \varphi'\right)\right]^{-1} e^{-2i\varphi} \tan\theta^q \tau^{qq'} \right]_{\beta\alpha} \\
&= e^{-2i\varphi} \sum_{\mu,\nu,\sigma>0} \tau^{qq'*}_{\mu\beta} \tau^{qq'}_{\nu\alpha} S_{\mu\sigma} S_{\nu\sigma} \tan\theta^q_{\nu} \\
&\times \frac{1 + D^{q'}_{\sigma\sigma} \cos(2\xi) - i D^{q'}_{\sigma\sigma} \sin(2\xi)}{1 + 2D^{q'}_{\sigma\sigma} \cos(2\xi) + \left(D^{q'}_{\sigma\sigma}\right)^2}
\end{aligned}
$$

where we have set $\xi = \varphi' - \varphi$. We can then define

$$W^{(+)}_{\beta\alpha}(\xi) \equiv \sum_{\mu,\nu,\sigma>0} \tau^{qq'*}_{\mu\beta} \tau^{qq'}_{\nu\alpha} S_{\mu\sigma} S_{\nu\sigma} \tan\theta^q_\nu \frac{\left[1 + D^{q'}_{\sigma\sigma}\cos(2\xi)\right]}{1 + 2D^{q'}_{\sigma\sigma}\cos(2\xi) + \left(D^{q'}_{\sigma\sigma}\right)^2} \tag{D.58}$$

$$Z^{(+)}_{\beta\alpha}(\xi) \equiv -\sum_{\mu,\nu,\sigma>0} \tau^{qq'*}_{\mu\beta} \tau^{qq'}_{\nu\alpha} S_{\mu\sigma} S_{\nu\sigma} \tan\theta^q_\nu \frac{D^{q'}_{\sigma\sigma}\sin(2\xi)}{1 + 2D^{q'}_{\sigma\sigma}\cos(2\xi) + \left(D^{q'}_{\sigma\sigma}\right)^2} \tag{D.59}$$

so that we can write the exponential form

$$\left[\tau^{qq'\dagger}\left[1 + M^q\left(\varphi,\varphi'\right)\right]^{-1} e^{-2i\varphi}\tan\theta^q \tau^{qq'}\right]_{\beta\alpha} = e^{-2i\varphi} n^{(+)}_{\beta\alpha}(\xi)\, e^{i\Omega^{(+)}_{\beta\alpha}(\xi)}$$

where

$$n^{(+)}_{\beta\alpha}(\xi) = \sqrt{\left[W^{(+)}_{\beta\alpha}(\xi)\right]^2 + \left[Z^{(+)}_{\beta\alpha}(\xi)\right]^2}$$

$$\Omega^{(+)}_{\beta\alpha}(\xi) = \tan^{-1}\left(W^{(+)}_{\beta\alpha}(\xi), Z^{(+)}_{\beta\alpha}(\xi)\right)$$

Putting all these results together, we find

$$\left\langle \Phi^{(p)}_q(\varphi) \left| a^{q'\dagger}_\alpha a^{q'\dagger}_{\bar\beta} \right| \Phi^{(p)}_{q'}\left(\varphi'\right)\right\rangle = e^{-2i\varphi}\left(\prod_{\mu>0} u^q_\mu u^{q'}_\mu\right) n(\xi)\, e^{i\Omega(\xi)} \times n^{(+)}_{\beta\alpha}(\xi)\, e^{i\Omega^{(+)}_{\beta\alpha}(\xi)} \tag{D.60}$$

As in the case of Eq. (D.55), and again because the operator $a^{q'\dagger}_\alpha a^{q'\dagger}_{\bar\beta}$ does not conserve particle number, we note that the matrix element does not depend on ξ alone. However, when Eqs. (D.55) and (D.60) are multiplied together, e.g. from the Wick-contracted form of a two-body term in the Hamiltonian, the troublesome factors $e^{2i\varphi'}$ and $e^{-2i\varphi}$ combine to give once again a dependence on ξ alone through the factor $e^{2i\xi}$. We also define the quantity

$$\begin{aligned} T_{\alpha\bar\beta}\left(\varphi,\varphi'\right) &\equiv \frac{\left\langle \Phi^{(p)}_q(\varphi)\left| a^{q'\dagger}_\alpha a^{q'\dagger}_{\bar\beta}\right| \Phi^{(p)}_{q'}\left(\varphi'\right)\right\rangle}{\left\langle \Phi^{(p)}_q(\varphi) \middle| \Phi^{(p)}_{q'}(\varphi')\right\rangle} \\ &= e^{-2i\varphi}\left[W^{(+)}_{\beta\alpha}(\xi) + iZ^{(+)}_{\beta\alpha}(\xi)\right] \end{aligned} \tag{D.61}$$

which will be useful in Sect. D.4.

D.4 Application to Hamiltonians

In this section we apply the formalism developed in this appendix to calculate non-diagonal matrix elements for a generic Hamiltonian, expressed in the basis at q'

$$\hat{H} = \sum_{\alpha\beta} \left\langle \alpha, q' \left| \hat{T} \right| \beta, q' \right\rangle a_\alpha^{q'\dagger} a_\beta^{q'} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \left\langle \alpha, q'; \beta, q' \left| \hat{V} \right| \gamma, \widetilde{q'; \delta, q'} \right\rangle a_\alpha^{q'\dagger} a_\beta^{q'\dagger} a_\delta^{q'} a_\gamma^{q'}$$

$$\equiv \sum_{\alpha\beta} T_{\alpha\beta}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\widetilde{\gamma\delta}}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'\dagger} a_\delta^{q'} a_\gamma^{q'}$$

For the one-body term, we use Eqs. (D.46) and (D.45) to write

$$\left\langle \Phi_q^{(p)}(\varphi) \left| \sum_{\alpha\beta} T_{\alpha\beta}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = \left(\prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) n(\xi)\, e^{i\Omega(\xi)} e^{2i\xi} \times 2 \sum_{\alpha,\beta>0} T_{\alpha\beta}^{q'} \left[W'_{\beta\alpha}(\xi) + i Z'_{\beta\alpha}(\xi) \right]$$

We can then define

$$W^{(0)}(\xi) \equiv 2 \sum_{\alpha,\beta>0} T_{\alpha\beta}^{q'} W'_{\beta\alpha}(\xi) \tag{D.62}$$

$$Z^{(0)}(\xi) \equiv 2 \sum_{\alpha,\beta>0} T_{\alpha\beta}^{q'} Z'_{\beta\alpha}(\xi) \tag{D.63}$$

and

$$W^{(0)}(\xi) + i Z^{(0)}(\xi) \equiv n^{(0)}(\xi)\, e^{i\Omega^{(0)}(\xi)} \tag{D.64}$$

to write

$$\left\langle \Phi_q^{(p)}(\varphi) \left| \sum_{\alpha\beta} T_{\alpha\beta}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = \left(\prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) n(\xi)\, e^{i\Omega(\xi)} e^{2i\xi} \times n^{(0)}(\xi)\, e^{i\Omega^{(0)}(\xi)}$$

Then the projected matrix element is

$$\left\langle \Phi_q^{(p)} \middle| P_q^{(N)\dagger} \left(\sum_{\alpha\beta} T_{\alpha\beta}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'} \right) P_{q'}^{(N)} \middle| \Phi_{q'}^{(p)} \right\rangle$$
$$= \frac{1}{\pi} \left(\prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) \int_0^\pi d\xi \, n(\xi) \, n^{(0)}(\xi) \times \cos\left[\Omega(\xi) + \Omega^{(0)}(\xi) - \xi(N-2) \right] \tag{D.65}$$

Next we calculate the contribution from the two-body term in the Hamiltonian. For compactness of notation we define the generalized density matrix elements equivalent to those given by Eqs. (4.5)–(4.7) in [1],

$$S_{\beta\alpha}(\varphi, \varphi') \equiv \frac{\left\langle \Phi_q^{(p)}(\varphi) \middle| a_\alpha^{q'\dagger} a_\beta^{q'} \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle}{\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle}$$

$$T_{\alpha\bar{\beta}}(\varphi, \varphi') \equiv \frac{\left\langle \Phi_q^{(p)}(\varphi) \middle| a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger} \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle}{\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle}$$

$$Y_{\alpha\bar{\beta}}(\varphi, \varphi') \equiv \frac{\left\langle \Phi_q^{(p)}(\varphi) \middle| a_\alpha^{q'} a_{\bar{\beta}}^{q'} \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle}{\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle}$$

We can use the generalized Wick's theorem given in Eq. (3.17) of [1] and obtain

$$\frac{1}{4} \left\langle \Phi_q^{(p)}(\varphi) \middle| \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\widetilde{\gamma\delta}}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'\dagger} a_\delta^{q'} a_\gamma^{q'} \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle$$
$$= \left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle$$
$$\times \left\{ \frac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\widetilde{\gamma\delta}}^{q'} S_{\gamma\alpha}(\varphi, \varphi') \, S_{\delta\beta}(\varphi, \varphi') \right.$$
$$\left. + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\bar{\beta}\widetilde{\gamma\bar{\delta}}}^{q'} T_{\alpha\bar{\beta}}(\varphi, \varphi') \, Y_{\bar{\delta}\gamma}(\varphi, \varphi') \right\}$$

Next, we use Eq. (D.47) to write

$$\sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\beta\widetilde{\gamma}\widetilde{\delta}} S_{\gamma\alpha}\left(\varphi,\varphi'\right) S_{\delta\beta}\left(\varphi,\varphi'\right)$$

$$= e^{4i\xi} \sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\beta\widetilde{\gamma}\widetilde{\delta}} \left[W'_{\gamma\alpha}(\xi) + iZ'_{\gamma\alpha}(\xi)\right]\left[W'_{\delta\beta}(\xi) + iZ'_{\delta\beta}(\xi)\right]$$

$$= e^{4i\xi}\left[W'(\xi) + iZ'(\xi)\right]$$

where we have defined

$$W'(\xi) \equiv \sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\beta\widetilde{\gamma}\widetilde{\delta}} \left[W'_{\gamma\alpha}(\xi)\, W'_{\delta\beta}(\xi) - Z'_{\gamma\alpha}(\xi)\, Z'_{\delta\beta}(\xi)\right] \tag{D.66}$$

$$Z'(\xi) \equiv \sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\beta\widetilde{\gamma}\widetilde{\delta}} \left[W'_{\gamma\alpha}(\xi)\, Z'_{\delta\beta}(\xi) + Z'_{\gamma\alpha}(\xi)\, W'_{\delta\beta}(\xi)\right] \tag{D.67}$$

For the remaining term in the two-body contribution, we use Eqs. (D.61) and (D.56) to write[2]

$$\sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\bar{\beta}\widetilde{\gamma}\widetilde{\bar{\delta}}} T_{\alpha\bar{\beta}}\left(\varphi,\varphi'\right) Y_{\bar{\delta}\gamma}\left(\varphi,\varphi'\right) = e^{2i\xi} \sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\bar{\beta}\widetilde{\gamma}\widetilde{\bar{\delta}}} \left[W^{(+)}_{\beta\alpha}(\xi) + iZ^{(+)}_{\beta\alpha}(\xi)\right]$$

$$\times\left[W^{(-)}_{\gamma\delta}(\xi) + iZ^{(-)}_{\gamma\delta}(\xi)\right]$$

$$= e^{2i\xi}\left[W^{(\pm)}(\xi) + iZ^{(\pm)}(\xi)\right]$$

where we have defined

$$W^{(\pm)}(\xi) \equiv \sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\bar{\beta}\widetilde{\gamma}\widetilde{\bar{\delta}}} \left[W^{(+)}_{\beta\alpha}(\xi)\, W^{(-)}_{\gamma\delta}(\xi) - Z^{(+)}_{\beta\alpha}(\xi)\, Z^{(-)}_{\gamma\delta}(\xi)\right] \tag{D.68}$$

$$Z^{(\pm)}(\xi) \equiv \sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\bar{\beta}\widetilde{\gamma}\widetilde{\bar{\delta}}} \left[W^{(+)}_{\beta\alpha}(\xi)\, Z^{(-)}_{\gamma\delta}(\xi) + Z^{(+)}_{\beta\alpha}(\xi)\, W^{(-)}_{\gamma\delta}(\xi)\right] \tag{D.69}$$

We are now ready to combine all the terms and project onto particle number for the Hamiltonian matrix elements,

$$\left\langle \Phi^{(p)}_q \left| P^{(N)\dagger}_q \hat{H} P^{(N)}_{q'} \right| \Phi^{(p)}_{q'} \right\rangle = \frac{1}{\pi}\left(\prod_{\mu>0} u^q_\mu u^{q'}_\mu\right) \int_0^\pi d\xi\, \mathrm{Re}\left\{e^{-i\xi N} n(\xi)\, e^{i\Omega(\xi)}\right.$$

$$\times\left\{e^{2i\xi}\left[W^{(0)}(\xi) + iZ^{(0)}(\xi)\right]\right.$$

[2]The sign in Eq. (D.56) does not appear because the order of indices is reversed in $Y_{\bar{\delta}\gamma}\left(\varphi,\varphi'\right)$.

$$+\frac{e^{4i\xi}}{2}\left[W'(\xi)+iZ'(\xi)\right]$$
$$+\frac{e^{2i\xi}}{4}\left[W^{(\pm)}(\xi)+iZ^{(\pm)}(\xi)\right]\Big\}\Big\}$$

We can then define

$$n_H(\xi)\,e^{i\Omega_H(\xi)} \equiv e^{2i\xi}\left[W^{(0)}(\xi)+iZ^{(0)}(\xi)\right]+\frac{e^{4i\xi}}{2}\left[W'(\xi)+iZ'(\xi)\right]$$
$$+\frac{e^{2i\xi}}{4}\left[W^{(\pm)}(\xi)+iZ^{(\pm)}(\xi)\right] \tag{D.70}$$

and obtain finally

$$\left\langle \Phi_q^{(p)} \middle| P_q^{(N)\dagger}\hat{H}P_{q'}^{(N)} \middle| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi}\left(\prod_{\mu>0} u_\mu^q u_\mu^{q'}\right)\int_0^\pi d\xi\, n(\xi)\, n_H(\xi) \tag{D.71}$$
$$\times \cos\left[\Omega(\xi)+\Omega_H(\xi)-N\xi\right]$$

which can be evaluated numerically.

Reference

1. Haider, Q., Gogny, D.: J. Phys. G **18**, 993 (1992)

Appendix E
Symmetric Ordered Products of Operators

E.1 Pedestrian Derivation of the SME

E.1.1 Basic Formula

Consider the integral

$$N(q) = \int_{-\infty}^{\infty} dq' \, N\left(q, q'\right) f\left(q'\right)$$

We change integration variable to $s = q - q'$,

$$N(q) = \int_{-\infty}^{\infty} ds \, N(q, q - s) \, f(q - s)$$

We expand $f(q - s)$ about q,

$$f(q - s) = \sum_{m=0}^{\infty} \frac{(-1)^m s^m}{m!} f^{(m)}(q)$$

and we expand

$$g(q) \equiv N(q, q - s)$$

about $q + s/2$,

$$g(q) = g\left(q + \frac{s}{2} - \frac{s}{2}\right)$$

W. Younes et al., *A Microscopic Theory of Fission Dynamics Based on the Generator Coordinate Method*, Lecture Notes in Physics 950,
https://doi.org/10.1007/978-3-030-04424-4

$$= \sum_{n=0}^{\infty} \frac{(-1)^n s^n}{2^n n!} g^{(n)}\left(q + \frac{s}{2}\right)$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^n s^n}{2^n n!} N^{(n)}\left(q + \frac{s}{2}, q - \frac{s}{2}\right)$$

Then we have

$$N(q) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(-1)^{m+n}}{2^n m! n!} f^{(m)}(q) \int_{-\infty}^{\infty} ds\, s^{m+n} N^{(n)}\left(q + \frac{s}{2}, q - \frac{s}{2}\right)$$

$$= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(-1)^{m+n}}{2^n m! n!} \left[\frac{\partial^m}{\partial q^m} f(q)\right]\left[\frac{\partial^n}{\partial q^n} \int_{-\infty}^{\infty} ds\, s^{m+n} N\left(q + \frac{s}{2}, q - \frac{s}{2}\right)\right]$$

Next, we gather terms with the same value of $m + n$. For this we define $p = m + n$ and write

$$N(q) = \sum_{p=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \delta_{m+n,p} \frac{(-1)^{m+n}}{2^n m! n!}$$

$$\times \left[\frac{\partial^m}{\partial q^m} f(q)\right]\left[\frac{\partial^n}{\partial q^n} \int_{-\infty}^{\infty} ds\, s^{m+n} N\left(q + \frac{s}{2}, q - \frac{s}{2}\right)\right]$$

$$= \sum_{p=0}^{\infty}\sum_{m=0}^{p} \frac{(-1)^p}{2^{p-m} m! (p-m)!}$$

$$\times \left[\frac{\partial^m}{\partial q^m} f(q)\right]\left[\frac{\partial^{p-m}}{\partial q^{p-m}} \int_{-\infty}^{\infty} ds\, s^p N\left(q + \frac{s}{2}, q - \frac{s}{2}\right)\right]$$

$$= \sum_{p=0}^{\infty} \frac{1}{p!}\frac{1}{2^p} \sum_{m=0}^{p} 2^m \binom{p}{m}$$

$$\times \left[i^m \frac{\partial^m}{\partial q^m} f(q)\right]\left[i^{p-m} \frac{\partial^{p-m}}{\partial q^{p-m}} i^p \int_{-\infty}^{\infty} ds\, s^p N\left(q + \frac{s}{2}, q - \frac{s}{2}\right)\right]$$

We then define

$$\hat{P} \equiv i \frac{\partial}{\partial q}$$

and

$$N_p(q) \equiv i^p \int_{-\infty}^{\infty} ds\, s^p N\left(q + \frac{s}{2}, q - \frac{s}{2}\right)$$

and, applying the definition of a SOPO given in Eq. (3.180),

$$\left[N_p(q)\,\hat{P}\right]^{(p)} f(q) \equiv \frac{1}{2^p}\sum_{m=0}^{p} 2^m \binom{p}{m} \left[\hat{P}^m f(q)\right]\left[\hat{P}^{p-m} N_p(q)\right] \tag{E.1}$$

so that

$$N(q) = \sum_{p=0}^{\infty} \frac{1}{p!}\left[N_p(q)\,\hat{P}\right]^{(p)}$$

We can check these results against for example the operator form in Eq. (3.180) for the order-2 case. From Eq. (3.180) we have

$$\begin{aligned}
\left[N^{(2)}(q)\,\hat{P}\right]^{(2)} f(q) &\equiv \frac{1}{2^2}\sum_{k=0}^{2}\binom{2}{k}\hat{P}^{2-k}N^{(2)}(q)\,\hat{P}^k f(q) \\
&= \frac{1}{4}\left\{\hat{P}^2 N^{(2)}(q) + 2\hat{P}N^{(2)}(q)\,\hat{P} + N^{(2)}(q)\,\hat{P}^2\right\} f(q) \\
&= \frac{1}{4}\left\{2^0 \times \left[\hat{P}^2 N^{(2)}(q)\right] + 2^1 \times 2\left[\hat{P}N^{(2)}(q)\right]\hat{P}\right. \\
&\quad \left. + 2^2 \times N^{(2)}(q)\,\hat{P}^2\right\} f(q)
\end{aligned}$$

where the square brackets have been added to make it clear that the operator $\hat{P}$ only acts within the brackets. Also the 2^m factor, which appears in Eq. (E.1) also appears here after combining common terms.

E.1.2 Derivatives of SOPOs

We derive a compact expression for

$$\begin{aligned}
\hat{P}^m\left\{\left[A(q)\,\hat{P}\right]^{(n)} f(q)\right\} &= \hat{P}^m \frac{1}{2^n}\sum_{k=0}^{n} 2^k \binom{n}{k}\left[\hat{P}^k f(q)\right]\left[\hat{P}^{n-k}A(q)\right] \\
&= \frac{1}{2^n}\sum_{k=0}^{n} 2^k \binom{n}{k}\sum_{l=0}^{m}\binom{m}{l} \\
&\quad \times \left[\hat{P}^{k+l} f(q)\right]\left[\hat{P}^{m+n-(k+l)}A(q)\right]
\end{aligned}$$

$$= \frac{1}{2^n} \sum_{r=0}^{\infty} \left[\sum_{k=0}^{n} 2^k \binom{n}{k} \binom{m}{r-k} \right] \times \left[\hat{P}^r f(q) \right] \left[\hat{P}^{m+n-r} A(q) \right]$$

Next, we wish to simplify the coefficient

$$C_{m,n,r} \equiv \sum_{k=0}^{n} 2^k \binom{n}{k} \binom{m}{r-k}$$

We use Mathematica to simplify this sum. If $m + 1 - r > 0$, then

$$C_{m,n,r} = \binom{m}{r} {}_2F_1(-n, -r; m + 1 - r; 2)$$

Otherwise, if $m + 1 - r \leq 0$,

$$C_{m,n,r} = 2^{r-m} \binom{n}{r-m} {}_2F_1(-m, -m - n - r; 1 - m + r; 2)$$

In either case,

$$\boxed{\hat{P}^m \left\{ \left[A(q)\, \hat{P} \right]^{(n)} f(q) \right\} = \frac{1}{2^n} \sum_{r=0}^{\infty} C_{m,n,r} \left[\hat{P}^r f(q) \right] \left[\hat{P}^{m+n-r} A(q) \right]} \qquad \text{(E.2)}$$

For example, for $m = 0$, we find for $r = 0$

$$C_{0,n,0} = 1$$

and for $r > 0$,

$$\begin{aligned} C_{0,n,r} &= 2^{r-m} \binom{n}{r-m} {}_2F_1(-m, -m - n - r; 1 - m + r; 2) \\ &= 2^r \binom{n}{r} {}_2F_1(0, -n - r; 1 + r; 2) \\ &= 2^r \binom{n}{r} \end{aligned}$$

and therefore,

$$\hat{P}^0\left\{\left[A(q)\,\hat{P}\right]^{(n)} f(q)\right\} = \frac{1}{2^n}\sum_{r=0}^{\infty} 2^r \binom{n}{r}\left[\hat{P}^r f(q)\right]\left[\hat{P}^{n-r}A(q)\right]$$
$$= \left[A(q)\,\hat{P}\right]^{(n)} f(q)$$

as expected.

E.1.2.1 Properties of the Coefficient $C_{m,n,r}$

We recall the definition,

$$C_{m,n,r} \equiv \sum_{k=0}^{n} 2^k \binom{n}{k}\binom{m}{r-k}$$

which reduces to

$$C_{m,n,r} = \begin{cases} \binom{m}{r}\,{}_2F_1\left(-n,-r;m+1-r;2\right) & m+1-r>0 \\ 2^{r-m}\binom{n}{r-m}\,{}_2F_1\left(-m,-m-n-r;1-m+r;2\right) & m+1-r\le 0 \end{cases}$$

Therefore we always have

$$C_{m,n,0} = \sum_{k=0}^{n} 2^k \binom{n}{k}\binom{m}{-k}$$

or,

$$\boxed{C_{m,n,0} = 1}$$

E.1.3 Useful Identities for SOPOs

First, for a generic operator A we write

$$\hat{P}A = A^{(1)} + A\hat{P}$$

or,

$$\boxed{A^{(1)} = \left[\hat{P}, A\right]} \tag{E.3}$$

Be careful not to confuse $A^{(1)}$ in this context with simple differentiation of the operator A.

In general, we can show by induction

$$\hat{P}^s A = \sum_{k=0}^{s} \binom{s}{k} A^{(s-k)} \hat{P}^k \tag{E.4}$$

For a generic operator A and integers $m \geq 0$ and $n \geq 0$ we next show that

$$\left(A \hat{P}^{(m)}\right)^{(n)} = A^{(n)} \hat{P}^{(m)}$$

We show this first for $n = 0$:

$$\begin{aligned}\left(A \hat{P}^{(m)}\right)^{(0)} &= A \hat{P}^{(m)} \\ &= A^{(0)} \hat{P}^{(m)}\end{aligned}$$

Next, we show that if the identity is true for n, then it is also true for $n + 1$ by using Eq. (E.3) to calculate

$$\begin{aligned}\left(A \hat{P}^{(m)}\right)^{(n+1)} &= \left(\left(A \hat{P}^{(m)}\right)^{(n)}\right)^{(1)} \\ &= \hat{P}\left(A^{(n)} \hat{P}^{(m)}\right) - \left(A^{(n)} \hat{P}^{(m)}\right) \hat{P} \\ &= A^{(n+1)} \hat{P}^{(m)}\end{aligned}$$

Therefore, by induction, we deduce

$$\boxed{\left(A \hat{P}^{(m)}\right)^{(n)} = A^{(n)} \hat{P}^{(m)}} \tag{E.5}$$

Next, we show that

$$\left(\hat{P}^{(m)} A\right)^{(n)} = \hat{P}^{(m)} A^{(n)}$$

Again, we start with the $n = 0$ case,

$$\begin{aligned}\left(\hat{P}^{(m)} A\right)^{(0)} &= \hat{P}^{(m)} A \\ &= \hat{P}^{(m)} A^{(0)}\end{aligned}$$

Next, we show that if the identity is true for n, then it is also true for $n+1$ by using Eq. (E.3) to calculate

$$\begin{aligned}\left(\hat{P}^{(m)}A\right)^{(n+1)} &= \left(\left(\hat{P}^{(m)}A\right)^{(n)}\right)^{(1)} \\ &= \hat{P}\left(\hat{P}^{(m)}A^{(n)}\right) - \left(\hat{P}^{(m)}A^{(n)}\right)\hat{P} \\ &= \hat{P}^{(m)}A^{(n+1)}\end{aligned}$$

Then, by induction, we deduce

$$\boxed{\left(\hat{P}^{(m)}A\right)^{(n)} = \hat{P}^{(m)}A^{(n)}} \tag{E.6}$$

Next we show that

$$A\hat{P}^{(n)} = \sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^{m}A^{(n-m)}$$

First we show this for $n = 0$. Trivially the LHS is

$$A\hat{P}^{(0)} = A$$

while the RHS is

$$\sum_{m=0}^{0}(-1)^{0-m}\binom{0}{m}\hat{P}^{m}A^{(0-m)} = A$$

as well. Then we assume the identity is true for n and deduce its validity for $n+1$ by calculating

$$A\hat{P}^{(n+1)} = \left[\sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^{m}A^{(n-m)}\right]\hat{P}$$

We then use Eq. (E.3) to write

$$\begin{aligned}A\hat{P}^{(n+1)} = &\left[\sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^{m+1}A^{(n-m)}\right] \\ &- \left(\sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^{m}A^{(n-m)}\right)^{(1)}\end{aligned}$$

and using Eq. (E.6) in the second term, this becomes

$$A\hat{P}^{(n+1)} = \sum_{m=0}^{n} (-1)^{n-m} \binom{n}{m} \hat{P}^{m+1} A^{(n-m)} - \sum_{m=0}^{n} (-1)^{n-m} \binom{n}{m} \hat{P}^{m} A^{(n-m+1)}$$

$$= \sum_{m=1}^{n+1} (-1)^{n-m+1} \binom{n}{m-1} \hat{P}^{m} A^{(n-m+1)} - \sum_{m=0}^{n} (-1)^{n-m} \binom{n}{m} \hat{P}^{m} A^{(n-m+1)}$$

$$= \sum_{m=0}^{n+1} (-1)^{n+1-m} \left[\binom{n}{m-1} + \binom{n}{m} \right] \hat{P}^{m} A^{(n+1-m)}$$

We can then use Pascal's rule for the binomial coefficients to write

$$A\hat{P}^{(n+1)} = \sum_{m=0}^{n+1} (-1)^{n+1-m} \binom{n+1}{m} \hat{P}^{m} A^{(n+1-m)}$$

which proves the induction step. Therefore we have established

$$\boxed{A\hat{P}^{(n)} = \sum_{m=0}^{n} (-1)^{n-m} \binom{n}{m} \hat{P}^{m} A^{(n-m)}} \tag{E.7}$$

Returning to SOPOs, we show that

$$\left(\left[B\hat{P} \right]^{(q)} \right)^{(s)} = \left[B^{(s)} \hat{P} \right]^{(q)}$$

To prove this, we write

$$\left(\left[B\hat{P} \right]^{(q)} \right)^{(s)} = \left(\frac{1}{2^q} \sum_{i=0}^{q} \binom{q}{i} \hat{P}^{q-i} B \hat{P}^{i} \right)^{(s)}$$

Using Eq. (E.5), this becomes

$$\left(\left[B\hat{P}\right]^{(q)}\right)^{(s)} = \frac{1}{2^q}\sum_{i=0}^{q}\binom{q}{i}\left(\hat{P}^{q-i}B\right)^{(s)}\hat{P}^i$$

and using Eq. (E.6), this reduces to

$$\left(\left[B\hat{P}\right]^{(q)}\right)^{(s)} = \frac{1}{2^q}\sum_{i=0}^{q}\binom{q}{i}\hat{P}^{q-i}B^{(s)}\hat{P}^i$$

or,

$$\boxed{\left(\left[B\hat{P}\right]^{(q)}\right)^{(s)} = \left[B^{(s)}\hat{P}\right]^{(q)}} \tag{E.8}$$

Next, we simplify the expression for

$$A\left[B\hat{P}\right]^{(q)} = A\frac{1}{2^q}\sum_{s=0}^{q}\binom{q}{s}\hat{P}^{q-s}B\hat{P}^s$$

Using Eq. (E.7), we write

$$\begin{aligned} A\left[B\hat{P}\right]^{(q)} &= \frac{1}{2^q}\sum_{s=0}^{q}\binom{q}{s}\left[\sum_{m=0}^{q-s}(-1)^{q-s-m}\binom{q-s}{m}\hat{P}^m A^{(q-s-m)}\right]B\hat{P}^s \\ &= \frac{1}{2^q}\sum_{s=0}^{q}\sum_{m=0}^{q-s}(-1)^{q-s-m}\binom{q}{s}\binom{q-s}{m}\hat{P}^m A^{(q-s-m)}B\hat{P}^s \end{aligned}$$

We introduce an index $t = q - s - m$, and use it to eliminate the sum over m,

$$\begin{aligned} A\left[B\hat{P}\right]^{(q)} &= \frac{1}{2^q}\sum_{t=0}^{\infty}\delta_{t,q-s-m}\sum_{s=0}^{q}\sum_{m=0}^{q-s}(-1)^{q-s-m}\binom{q}{s}\binom{q-s}{m} \\ &\quad \times \hat{P}^m A^{(q-s-m)}B\hat{P}^s \\ &= \frac{1}{2^q}\sum_{t=0}^{\infty}\sum_{s=0}^{q}(-1)^t\binom{q}{s}\binom{q-s}{q-s-t}\hat{P}^{q-s-t}A^{(t)}B\hat{P}^s \end{aligned}$$

The product of the two binomial coefficients can be re-written

$$A\left[B\hat{P}\right]^{(q)} = \frac{1}{2^q}\sum_{t=0}^{\infty}\sum_{s=0}^{q}(-1)^t\binom{q}{t}\binom{q-t}{s}\hat{P}^{q-s-t}A^{(t)}B\hat{P}^s$$

$$= \frac{1}{2^q}\sum_{t=0}^{q}(-1)^t\binom{q}{t}\left[\sum_{s=0}^{q-t}\binom{q-t}{s}\hat{P}^{q-s-t}A^{(t)}B\hat{P}^s\right]$$

Using Eq. (3.180), the term in brackets can be written as a SOPO, and we get

$$A\left[B\hat{P}\right]^{(q)} = \frac{1}{2^q}\sum_{t=0}^{q}(-1)^t\binom{q}{t}2^{q-t}\left[A^{(t)}B\hat{P}\right]^{(q-t)}$$

or,

$$\boxed{A\left[B\hat{P}\right]^{(q)} = \sum_{t=0}^{q}\left(-\frac{1}{2}\right)^t\binom{q}{t}\left[A^{(t)}B\hat{P}\right]^{(q-t)}} \tag{E.9}$$

We can also show that

$$\left[A\hat{P}\right]^{(n)}B = \sum_{s=0}^{n}\frac{1}{2^s}\binom{n}{s}\left[AB^{(s)}P\right]^{(n-s)}$$

To prove this, we start with Eq. (3.180) and write

$$\left[A\hat{P}\right]^{(n)}B = \frac{1}{2^n}\sum_{r=0}^{n}\binom{n}{r}\hat{P}^{n-r}A\hat{P}^rB$$

Then we use Eq. (E.4),

$$\left[A\hat{P}\right]^{(n)}B = \frac{1}{2^n}\sum_{r=0}^{n}\binom{n}{r}\hat{P}^{n-r}A\sum_{i=0}^{r}\binom{r}{i}B^{(r-i)}P^i$$

$$= \frac{1}{2^n}\sum_{r=0}^{n}\sum_{i=0}^{r}\binom{n}{r}\binom{r}{i}\hat{P}^{n-r}AB^{(r-i)}P^i$$

We introduce the summing index $s = r - i$, and use it to replace the sum over r

$$\left[A\hat{P}\right]^{(n)} B = \frac{1}{2^n}\sum_{s=0}^{\infty}\sum_{r=0}^{n}\sum_{i=0}^{r}\binom{n}{r}\binom{r}{i}\delta_{s,r-i}\,\hat{P}^{n-r}AB^{(r-i)}P^i$$
$$= \frac{1}{2^n}\sum_{s=0}^{\infty}\sum_{i=0}^{n}\binom{n}{s+i}\binom{s+i}{i}\hat{P}^{n-s-i}AB^{(s)}P^i$$

Writing out the binomial coefficients in terms of factorials, we can readily show

$$\binom{n}{s+i}\binom{s+i}{i} = \binom{n}{s}\binom{n-s}{i}$$

so that

$$\left[A\hat{P}\right]^{(n)} B = \frac{1}{2^n}\sum_{s=0}^{\infty}\sum_{i=0}^{n}\binom{n}{s}\binom{n-s}{i}\hat{P}^{n-s-i}AB^{(s)}P^i$$
$$= \frac{1}{2^n}\sum_{s=0}^{n}\binom{n}{s}2^{n-s}\frac{1}{2^{n-s}}\sum_{i=0}^{n}\binom{n-s}{i}\hat{P}^{n-s-i}AB^{(s)}P^i$$

and using Eq. (3.180) again, we can write this as

$$\boxed{\left[A\hat{P}\right]^{(n)} B = \sum_{s=0}^{n}\frac{1}{2^s}\binom{n}{s}\left[AB^{(s)}P\right]^{(n-s)}} \tag{E.10}$$

Next, we show that

$$\left[\left[A\hat{P}\right]^{(n)}\hat{P}\right]^{(q)} = \left[A\hat{P}\right]^{(n+q)}$$

Using Eq. (3.180) we write

$$\left[\left[A\hat{P}\right]^{(n)}\hat{P}\right]^{(q)} = \frac{1}{2^q}\sum_{i=0}^{q}\binom{q}{i}\hat{P}^{q-i}\left[A\hat{P}\right]^{(n)}\hat{P}^i$$

and use Eq. (3.180) again to write

$$\left[\left[A\hat{P}\right]^{(n)}\hat{P}\right]^{(q)} = \frac{1}{2^q}\sum_{i=0}^{q}\binom{q}{i}\hat{P}^{q-i}\left[\frac{1}{2^n}\sum_{j=0}^{n}\binom{n}{j}\hat{P}^{n-j}A\hat{P}^j\right]\hat{P}^i$$
$$= \frac{1}{2^{n+q}}\sum_{i=0}^{q}\sum_{j=0}^{n}\binom{q}{i}\binom{n}{j}\hat{P}^{q-i+n-j}A\hat{P}^{i+j}$$

We introduce a new summation index $s = i + j$ and use it to replace the summation over j,

$$\left[\left[A\hat{P}\right]^{(n)}\hat{P}\right]^{(q)} = \frac{1}{2^{n+q}}\sum_{s=0}^{\infty}\delta_{s,i+j}\sum_{i=0}^{q}\sum_{j=0}^{n}\binom{q}{i}\binom{n}{j}\hat{P}^{q-i+n-j}A\hat{P}^{i+j}$$
$$= \frac{1}{2^{n+q}}\sum_{s=0}^{n+q}\sum_{i=0}^{s}\binom{q}{i}\binom{n}{s-i}\hat{P}^{q+n-s}A\hat{P}^{s}$$

Where the sum over s stops at $n+q$ since that is the largest possible value of $i+j$, and the upper limit of the sum over i has been changed to s since the maximum value of s is $n+q$, which includes q. The sum over i can be further simplified using the Chu-Vandermonde identity,

$$\sum_{i=0}^{s}\binom{q}{i}\binom{n}{s-i} = \binom{n+q}{s}$$

Therefore,

$$\left[\left[A\hat{P}\right]^{(n)}\hat{P}\right]^{(q)} = \frac{1}{2^{n+q}}\sum_{s=0}^{n+q}\binom{n+q}{s}\hat{P}^{q+n-s}A\hat{P}^{s}$$

Using Eq. (3.180) one final time, we get

$$\boxed{\left[\left[A\hat{P}\right]^{(n)}\hat{P}\right]^{(q)} = \left[A\hat{P}\right]^{(n+q)}} \tag{E.11}$$

E.1.4 Composition of Two SOPOs

We use Eq. (E.10) to write

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} = \sum_{s=0}^{n}\frac{1}{2^{s}}\binom{n}{s}\left[A\left(\left[B\hat{P}\right]^{(q)}\right)^{(s)}P\right]^{(n-s)}$$

and use Eq. (E.8),

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} = \sum_{s=0}^{n}\frac{1}{2^s}\binom{n}{s}\left[A\left[B^{(s)}\hat{P}\right]^{(q)}P\right]^{(n-s)}$$

Next, we use Eq. (E.9),

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} = \sum_{s=0}^{n}\frac{1}{2^s}\binom{n}{s}\sum_{t=0}^{q}\left(-\frac{1}{2}\right)^t\binom{q}{t}\left[\left[A^{(t)}B^{(s)}\hat{P}\right]^{(q-t)}P\right]^{(n-s)}$$

Using Eq. (E.11), this becomes

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} = \sum_{s=0}^{n}\sum_{t=0}^{q}\frac{(-1)^t}{2^{s+t}}\binom{n}{s}\binom{q}{t}\left[A^{(t)}B^{(s)}\hat{P}\right]^{(n+q-s-t)}$$

At this point, we introduce a new summation variable $i = s + t$, and use it to eliminate the sum over t:

$$\begin{aligned}\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} &= \sum_{i=0}^{\infty}\delta_{i,s+t}\sum_{s=0}^{n}\sum_{t=0}^{q}\frac{(-1)^t}{2^{s+t}}\binom{n}{s}\binom{q}{t}\left[A^{(t)}B^{(s)}\hat{P}\right]^{(n+q-s-t)}\\ &= \sum_{i=0}^{\infty}\sum_{s=0}^{n}\frac{(-1)^{i-s}}{2^i}\binom{n}{s}\binom{q}{i-s}\left[A^{(i-s)}B^{(s)}\hat{P}\right]^{(n+q-i)}\end{aligned}$$

To complete the derivation, we give more stringent limits for the summation indices i and s. The binomial coefficients impose the conditions

$$\begin{aligned}0 \le \quad s \quad &\le n\\ 0 \le i - s &\le q\end{aligned}$$

Thus we have

$$i \le s + q \le n + q$$

while for s, we have the two inequality relations

$$\begin{aligned}0 \le s \le n\\ i - q \le s \le i\end{aligned}$$

which we can combine into a single one,

$$\max(0, i - q) \le s \le \min(i, n)$$

Therefore, we have shown

$$\boxed{\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}=\sum_{i=0}^{n+q}\sum_{s=\max(0,i-q)}^{\min(i,n)}\frac{(-1)^{i-s}}{2^i}\binom{n}{s}\binom{q}{i-s}\times\left[A^{(i-s)}B^{(s)}\hat{P}\right]^{(n+q-i)}} \tag{E.12}$$

which gives the composition of two SOPO's as a linear combination of SOPO's.

E.1.5 Composition of Three SOPO's

Using Eq. (E.12) we write

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}\left[C\hat{P}\right]^{(r)}=\left[A\hat{P}\right]^{(n)}\sum_{i=0}^{q+r}\sum_{s=\max(0,i-r)}^{\min(i,q)}\frac{(-1)^{i-s}}{2^i}\binom{q}{s}\binom{r}{i-s}\times\left[B^{(i-s)}C^{(s)}\hat{P}\right]^{(q+r-i)}$$

and we use Eq. (E.12) again to write

$$\begin{aligned}\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}\left[C\hat{P}\right]^{(r)}=&\sum_{i=0}^{q+r}\sum_{s=\max(0,i-r)}^{\min(i,q)}\frac{(-1)^{i-s}}{2^i}\binom{q}{s}\binom{r}{i-s}\\&\sum_{j=0}^{n+q+r-i}\sum_{t=\max(0,j-(q+r-i))}^{\min(j,n)}\frac{(-1)^{j-t}}{2^j}\binom{n}{t}\\&\times\binom{q+r-i}{j-t}\left[A^{(j-t)}\left(B^{(i-s)}C^{(s)}\right)^{(t)}\hat{P}\right]^{(n+q+r-i-j)}\end{aligned}$$

To simplify the notation, we collect all the terms that depend on s into a single term

$$F(B,C,r,i,t)\equiv\sum_{s=\max(0,i-r)}^{\min(i,q)}(-1)^s\binom{q}{s}\binom{r}{i-s}\left(B^{(i-s)}C^{(s)}\right)^{(t)} \tag{E.13}$$

so that

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}\left[C\hat{P}\right]^{(r)} = \sum_{i=0}^{q+r}\frac{(-1)^i}{2^i}\sum_{j=0}^{n+q+r-i}\sum_{t=\max(0,j-(q+r-i))}^{\min(j,n)}\frac{(-1)^{j-t}}{2^j}$$
$$\times\binom{n}{t}\binom{q+r-i}{j-t}$$
$$\times\left[A^{(j-t)}F\left(B,C,r,i,t\right)\hat{P}\right]^{(n+q+r-i-j)}$$

Next, we introduce a sum over $p = i + j$ to eliminate the sum over j,

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}\quad\left[C\hat{P}\right]^{(r)} = \sum_{p=0}^{\infty}\sum_{i=0}^{q+r}\frac{(-1)^i}{2^i}\sum_{t=\max(0,p-(q+r))}^{\min(p-i,n)}\frac{(-1)^{p-i-t}}{2^{p-i}}\binom{n}{t}$$
$$\times\binom{q+r-i}{p-i-t}\left[A^{(p-i-t)}F\left(B,C,r,i,t\right)\hat{P}\right]^{(n+q+r-p)}$$
$$= \sum_{p=0}^{\infty}\sum_{i=0}^{q+r}\frac{(-1)^p}{2^p}\sum_{t=\max(0,p-(q+r))}^{\min(p-i,n)}(-1)^t\binom{n}{t}$$
$$\times\binom{q+r-i}{p-i-t}\left[A^{(p-i-t)}F\left(B,C,r,i,t\right)\hat{P}\right]^{(n+q+r-p)}$$

To complete the derivation, we give more stringent limits for the summation indices p and i. From the binomial coefficients we see that

$$i \leq q + r$$

but also

$$i \leq p - t \leq p$$

and therefore,

$$i \leq \min\left(p, q + r\right)$$

Finally,

$$p - i - t \leq q + r - i$$
$$\Rightarrow p \leq q + r + t$$

but since $t \leq n$, then we must have

$$p \leq q + r + n$$

In summary, we have shown

$$\boxed{\begin{aligned}\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}\left[C\hat{P}\right]^{(r)} = \sum_{p=0}^{n+q+r}\sum_{i=0}^{\min(p,q+r)}\frac{(-1)^p}{2^p}\sum_{t=\max(0,p-q-r)}^{\min(p-i,n)}(-1)^t \\ \times\binom{n}{t}\binom{q+r-i}{p-i-t} \\ \times\left[A^{(p-i-t)}F\left(B,C,r,i,t\right)\hat{P}\right]^{(n+q+r-p)}\end{aligned}} \tag{E.14}$$

which gives the composition of three SOPO's as a linear combination of SOPO's.

E.1.5.1 Special Cases

We derive here Eqs. (A5) and (A6) in [1]. Using Eq. (E.14) with $n = r = 0$ and $q = 1$ we get

$$\begin{aligned}A\left[B\hat{P}\right]^{(1)}C &= \sum_{p=0}^{1}\sum_{i=0}^{p}\frac{(-1)^p}{2^p}\binom{1-i}{p-i}\left[A^{(p-i)}F\left(B,C,0,i,0\right)\hat{P}\right]^{(1-p)} \\ &= \left[AF\left(B,C,0,0,0\right)\hat{P}\right]^{(1)} - \frac{1}{2}\left\{A^{(1)}F\left(B,C,0,0,0\right)\right. \\ &\left.+AF\left(B,C,0,1,0\right)\right\}\end{aligned}$$

Now, using Eq. (E.13),

$$F\left(B,C,0,i,0\right) = (-1)^i\binom{q}{i}BC^{(i)}$$

and in particular,

$$F\left(B,C,0,0,0\right) = BC$$

and

$$F\left(B,C,0,1,0\right) = -BC^{(1)}$$

and therefore

$$\boxed{A\left[B\hat{P}\right]^{(1)}C = \left[ABC\hat{P}\right]^{(1)} + \frac{1}{2}\left(ABC^{(1)} - A^{(1)}BC\right)} \tag{E.15}$$

Next, using Eq. (E.14) with $n = r = 0$ and $q = 2$ we get

$$A\left[B\hat{P}\right]^{(2)}C = \sum_{p=0}^{2}\sum_{i=0}^{p}\frac{(-1)^p}{2^p}\binom{2-i}{p-i}\left[A^{(p-i)}F\left(B,C,0,i,0\right)\hat{P}\right]^{(2-p)}$$
$$= \left[AF\left(B,C,0,0,0\right)\hat{P}\right]^{(2)} - \frac{1}{2}\left\{2\left[A^{(1)}F\left(B,C,0,0,0\right)\hat{P}\right]^{(1)}\right.$$
$$\left.+\left[AF\left(B,C,0,1,0\right)\hat{P}\right]^{(1)}\right\} + \frac{1}{4}\left\{A^{(2)}F\left(B,C,0,0,0\right)\right.$$
$$\left.+A^{(1)}F\left(B,C,0,1,0\right) + AF\left(B,C,0,2,0\right)\right\}$$

or,

$$A\left[B\hat{P}\right]^{(2)}C = \left[ABC\hat{P}\right]^{(2)} + \left[\left(ABC^{(1)} - A^{(1)}BC\right)\hat{P}\right]^{(1)} + \frac{1}{4}\left(A^{(2)}BC - 2A^{(1)}BC^{(1)} + ABC^{(2)}\right) \tag{E.16}$$

Next, we look at the special case where

$$A = C = \frac{1}{\sqrt{N^{(0)}}}$$

Then, using Eq. (E.15) we get

$$\frac{1}{\sqrt{N^{(0)}}}\left[B\hat{P}\right]^{(1)}\frac{1}{\sqrt{N^{(0)}}} = \left[\bar{B}\hat{P}\right]^{(1)} + \frac{i}{2}C^{(1)}\left(B, N^{(0)}\right) \tag{E.17}$$

where

$$\bar{B} \equiv \frac{1}{\sqrt{N^{(0)}}}B\frac{1}{\sqrt{N^{(0)}}}$$
$$C^{(1)}\left(B, N^{(0)}\right) \equiv \frac{1}{\sqrt{N^{(0)}}}B\left(\frac{1}{\sqrt{N^{(0)}}}\right)' - \left(\frac{1}{\sqrt{N^{(0)}}}\right)'B\frac{1}{\sqrt{N^{(0)}}}$$

Next, using Eq. (E.16),

$$\frac{1}{\sqrt{N^{(0)}}}\left[B\hat{P}\right]^{(2)}\frac{1}{\sqrt{N^{(0)}}} = \left[\bar{B}\hat{P}\right]^{(2)} + \left[iC^{(1)}\left(B, N^{(0)}\right)\hat{P}\right]^{(1)} - C^{(2)}\left(B, N^{(0)}\right) \tag{E.18}$$

where

$$C^{(2)}\left(B, N^{(0)}\right) \equiv \frac{1}{4}\left[\left(\frac{1}{\sqrt{N^{(0)}}}\right)'' B \frac{1}{\sqrt{N^{(0)}}} - 2\left(\frac{1}{\sqrt{N^{(0)}}}\right)' B \left(\frac{1}{\sqrt{N^{(0)}}}\right)' \right.$$
$$\left. + \frac{1}{\sqrt{N^{(0)}}} B \left(\frac{1}{\sqrt{N^{(0)}}}\right)''\right]$$

Reference

1. Bernard, R., Goutte, H., Gogny, D., Younes, W.: Phys. Rev. C **84**, 044308 (2011)

Appendix F
Algorithm for the TDGCM in the Gaussian Overlap Approximation

The algorithm used in this manuscript for the time-dependent generator-coordinate method in the Gaussian overlap approximation was discussed in [1, 2], and continues to be improved upon [3]. We give the broad outline of the algorithm here for convenience, and direct the reader to [2] in particular for more details.

Algorithm 2 gives the pseudocode for the main algorithm, and the Crank-Nicholson algorithm [2, 4] used to evolve the wave function in time is given in Algorithm 3. The main algorithm in Algorithm 2 begins by reading in the potential energy surface with zero-point energy corrections ($V(q_{20}, q_{30})$, if the HFB calculations are constrained by the quadrupole and octupole moments, for example) in Step 1 and the components of the inertia tensor ($B_{22}(q_{20}, q_{30})$, $B_{23}(q_{20}, q_{30})$, $B_{33}(q_{20}, q_{30})$) in Step 2. The collective Hamiltonian on the discretized (q_{20}, q_{30}) grid, $K(q_{20}, q_{30})$, is constructed in Step 3. The construction of $K(q_{20}, q_{30})$ involves replacing the derivatives in the expression for the collective Hamiltonian (see Sect. 3.2.1),

$$H_{\text{coll}} = -\frac{\hbar^2}{2} \sum_{i,j=2}^{3} \frac{\partial}{\partial q_{i0}} B_{ij}(q_{20}, q_{30}) \frac{\partial}{\partial q_{i0}} + V(q_{20}, q_{30}) \quad \text{(F.1)}$$

with their finite difference approximations. Explicit expressions for $K(q_{20}, q_{30})$ can be found in the appendix of [2]. The initial wave function, $g(t = 0)$, usually generated by the solution to the static GCM equation, is read into memory in Step 4. At this point, the time evolution loop of the TDGCM algorithm begins. At each time increment Δt, the Crank-Nicholson algorithm given in Algorithm 3 is applied to evolve $g(t)$ into $g(t + \Delta t)$ at Step 6. In order to avoid reflections of the wave function at the far end of the (q_{20}, q_{30}) grid (i.e., at very large values of q_{20}) the wave function $g(t + \Delta t)$ is multiplied by a damping factor with a Woods-Saxon form (see, e.g., Eq. (24) in [2]) in Step 7. The loop repeats until the user-supplied termination time $t_{\max}$.

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Algorithm 2 Pseudocode for the TDGCM algorithm

Read PES
Read inertia tensor
Construct collective Hamiltonian K
Read initial wave function
for $t = 0$ to t_{max} by Δt **do**
    Apply Crank-Nicholson algorithm to wave function
    Damp wave function
end for

Algorithm 3 Crank-Nicholson algorithm

Initialize wave function gn0 $\leftarrow g(t)$
repeat
    gn1 $\leftarrow g(t) - \frac{i\Delta t}{2\hbar} K g(t) - \frac{i\Delta t}{2\hbar} K$ gn0
    $\epsilon \leftarrow \sup|\text{gn1} - \text{gn0}|$
    gn0 $\leftarrow$ gn1
until $\epsilon > \epsilon_{\text{max}}$ or too many iterations

References

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3. Regnier, D., Dubray, N., Verrière, M., Schunck, N.: Comput. Phys. Commun. **225**, 180 (2018)
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Appendix G
Mathematica Script for Calculating the Coefficients of the Schrodinger-Like Equation

The following Mathematica (Wolfram Research [1]) script implements the SOPO algebra used to simplify expressions in Chap. 3.

```
Unprotect[NonCommutativeMultiply];
(* zero element *)
0**A_ := 0; A_**0 := 0;
(* unit element *)
1**A_ := A; A_**1 := A;
(* distributivity *)
A_**(B_+C_) := A**B + A**C; (B_+C_)**A_ := B**A + C**A;
(* product with a scalar *)
number3Q[x_,y_,n_] := NumberQ[x]&&NumberQ[y]&&NumberQ[n
    ];
A_**(B_(x_.y_^n_./;number3Q[x,y,n])) := ((x*y^n)A**B);
    (A_(x_.y_^n_./;number3Q[x,y,n]))**B_ := ((x*y^n)A**B
    );
(* Composition of three SOPO's *)
sopo[n_][A_]**sopo[q_][B_]**sopo[r_][C_] := Module[ {
    i,imax,p,t,tmin,tmax,F,s,smin,smax,val},  val = 0;
For[p = 0, p <= n+q+r, p++,
     imax = Min[p,q+r];
     For[i = 0, i <= imax, i++,
        tmin = Max[0,p-q-r];
        tmax = Min[p-i,n];
        For[t = tmin, t <= tmax, t++,
           F = 0;
           smin = Max[0,i-r];
           smax = Min[i,q];
           For[s = smin, s <= smax, s++,
```


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```
          F += I^(i+t)*(-1)^s*Binomial[q,s]*Binomial[r,
             i-s]*Derivative[t][Derivative[i-s][B]**
             Derivative[s][C]];          ];
        val += I^(p-i-t)*(-1)^(p+t)/2^p*Binomial[n,t]*
           Binomial[q+r-i,p-i-t]*sopo[n+q+r-p][
           Derivative[p-i-t][A]**F];          ];
    ];
  ];
  val ];
(* Composition of two SOPO's *)
sopo[n_][A_]**sopo[q_][B_] := Module[  {i,s,smin,smax,
   val},  val = 0;  For[i = 0, i <= n+q, i++,
   smin = Max[0,i-q];   smax = Min[i,n];   For[s =
   smin, s <= smax, s++,      val += I^i*(-1)^(i-s)/2^
   i*Binomial[n,s]*Binomial[q,i-s]*sopo[n+q-i][
   Derivative[i-s][A]**Derivative[s][B]];    ];   ];
  val ];
Protect[NonCommutativeMultiply];
(* Derivatives of SOPO's *)
Unprotect[Derivative];
Derivative[q_][sopo[n_][A_]] := I^q*sopo[n][Derivative[
   q][A]];
Unprotect[NonCommutativeMultiply];
Derivative[q_][A_**B_] := Sum[Binomial[q,i]*Derivative[
   i][A]**Derivative[q-i][B],{i,0,q}];
Protect[NonCommutativeMultiply];
Protect[Derivative];
(* Some additional identities for SOPO's *)
sopo[n_][0] := 0;
sopo[q_][sopo[n_][A_]] := sopo[n+q][A];
sopo[n_][A_+B_] := sopo[n][A] + sopo[n][B];
sopo[q_][(x_.y_^n_./;number3Q[x,y,n])A_] := (x*y^n)sopo
   [q][A];
getcoeff[n_,expr_] := Module[  {term1,term11,term12,
   term13,out1},   term1 = Cases[expr,x_.sopo[n][A_]:>{
   x,A}];
  term11 = Cases[term1,{_,A_/;FreeQ[A,_**_]}];   term12
     = Cases[term1,{_,A_**B_/;(FreeQ[A,_**_]&&FreeQ[B,
     _**_])}];   term13 = Cases[term1,{_,A_**B_**X_/;(
     FreeQ[A,_**_]&&FreeQ[B,_**_]&&FreeQ[X,_**_])}];
  out1 = term11;    ];
(*****)
jop = 1 + sopo[1][j1] + sopo[2][j2]; hop = sopo[0][h0]
   + sopo[1][h1] + sopo[2][h2];
```

```
res = jop**hop**jop;
res1 = res; res1 = res1/.(sopo[n_][_]/;n>=3)->0
res1 = Collect[Simplify[res1],sopo[_][_]];
coeff0 = Plus@@Cases[res1,x_.sopo[0][A_]:>(x)A]; coeff1
    = Plus@@Cases[res1,x_.sopo[1][A_]:>(x)A]; coeff2 =
    Plus@@Cases[res1,x_.sopo[2][A_]:>(x)A];
(* Rules for making the notation more compact using:
    CP[A,B] = AB + BA    CM[A,B] = AB − BA    CP[A,B,C] =
    ABC + CBA    CM[A,B,C] = ABC − CBA *)
compactify = { y_.A_**B_ + z_.B_**A_/;z == y :> (y)CP[A
    ,B], y_.A_**B_ + z_.B_**A_/;z == −y :> (y)CM[A,B],
    y_.A_**B_**F_ + z_.F_**B_**A_/;z == y :> (y)CP[A,B,
    F], y_.A_**B_**F_ + z_.F_**B_**A_/;z == −y :> (y)CM
    [A,B,F] };
coeffS = coeff0//.compactify; coeffT = coeff1//.
    compactify; coeffU = coeff2//.compactify;
```

Reference

1. Wolfram Research, Inc.: Mathematica Version 9.0. Wolfram Research Inc., Champaign (2012)

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