Gaussian matrix elements in a cylindrical harmonic oscillator basis

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Abstract

We derive a formalism, the separation method, for the efficient and accurate calculation of two-body matrix elements for a Gaussian potential in the cylindrical harmonic-oscillator basis. This formalism is of critical importance for Hartree-Fock and Hartree-Fock-Bogoliubov calculations in deformed nuclei using realistic, finite-range effective interactions between nucleons. The results given here are also relevant for microscopic many-body calculations in atomic and molecular physics, as the formalism can be applied to other types of interactions beyond the Gaussian form. The derivation is presented in great detail to emphasize the methodology, which relies on generating functions. The resulting analytical expressions for the Gaussian matrix elements are checked for speed and accuracy as a function of the number of oscillator shells and against direct numerical integration.

Key words: Deformed harmonic oscillator, Gaussian interaction, Matrix elements, Gogny force
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1 Introduction

Gaussian interactions play an important role in the microscopic description of molecular and nuclear processes [1]. The Gaussian form represents a relatively simple two-body potential with a finite range, which is needed in many realistic descriptions of many-body systems. In nuclear physics for example, the Gogny interaction [2]

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$$
\begin{aligned}
V\left(\vec{r}_1, \vec{r}_2\right) = & \sum_{i=1}^{2}\left(W_i + B_i \hat{P}_\sigma - H_i \hat{P}_\tau - M_i \hat{P}_\sigma \hat{P}_\tau\right) e^{-\left(\vec{r}_1-\vec{r}_2\right)^2/\mu_i^2} \\
& + i W_{LS}\left(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2\right) \times \delta\left(\vec{r}_1 - \vec{r}_2\right)\left(\overrightarrow{\nabla}_1 - \overrightarrow{\nabla}_2\right) \cdot \left(\vec{\sigma}_1 + \vec{\sigma}_2\right) \\
& + t_0\left(1 + x_0 \hat{P}_\sigma\right) \delta\left(\vec{r}_1 - \vec{r}_2\right) \rho^\gamma\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right) + V_{\text{Coul}}
\end{aligned} \tag{1}
$$

where $\hat{P}_\sigma$ and $\hat{P}_\tau$ are spin- and isospin-exchange operators and ρ is the total nuclear density, gives the effective (in-medium) potential between nucleons. Two Gaussian terms appear explicitly with range parameters μ_1 and μ_2. A spin-orbit term with strength W_{LS} uses a Dirac-delta function, but extensions of the Gogny force have been proposed [3] that introduce a Gaussian form for this term. Finally the Coulomb interaction $V_{\text{Coul}} \sim 1/\left|\vec{r}_1 - \vec{r}_2\right|$ between protons is clearly not of Gaussian form, but the mathematical framework presented in this paper can be applied equally well to a Coulomb potential.

For the calculation of matrix elements in molecular, atomic, and nuclear physics, harmonic-oscillator functions provide a convenient and popular orthogonal basis. The calculation of Gaussian matrix elements in a harmonic-oscillator basis, however, poses definite technical challenges in accuracy as well as execution time. In previous work [4], the separation method was introduced as a way of calculating the Gaussian matrix elements efficiently and accurately for systems with spherical symmetry. In the separation method, two-body matrix elements are expressed as a more manageable finite sum of products of one-body matrix elements. In this paper, we derive the separation method for a wider class of systems that exhibit axial symmetry. These results are crucial, for example, in microscopic calculations of nuclear fission using the Gogny force, where the nucleus elongates along a symmetry axis, until scission occurs.

Fission calculations in particular bring to the fore many of the technical difficulties involved in the computation of Gaussian matrix elements. On the other hand, microscopic calculations of fission using the interaction in Eq. (1) have had considerable success in recent years [5,6,7], and are therefore of great interest. In the microscopic description of fission, the matrix elements of the nucleon-nucleon interaction are typically used in a Hartree-Fock-Bogoliubov (HFB) procedure to construct a Slater-determinant wave function for the nucleus. Scission configurations are then found by driving the nucleus to such exotic shapes that the delicate balance between its surface tension and the Coulomb repulsion between the nascent fission fragments is broken. The proper identification of scission configurations and the calculation of their properties depend sensitively on accurate calculations of the matrix elements of the effective interaction. Fission also implies the evolution of the nucleus through a variety of exotic shapes leading to scission. Therefore many sets of matrix elements need to be calculated, each set corresponding to a harmonic-oscillator basis optimized for a particular nuclear shape, and each set requiring a large number of oscillator shells. The resulting large-scale computations can become very time-consuming and are prone to errors in accuracy. Thus microscopic fission calculations must rely on fast and accurate algorithms to evaluate the two-body matrix elements, such as the separation method. The separation method is especially well-suited to the HFB algorithm, because the coefficients needed to calculate the two-body matrix elements derived in this paper can be calculated quickly once and for all, and stored with relatively little computer memory.

The goal of this paper is to derive the separation-method formalism for Gaussian matrix elements in a cylindrical harmonic-oscillator basis, with particular emphasis placed on the details of the derivation because of its relevance to other types of interactions, and other applications involving the harmonic-oscillator basis. In particular, we rely heavily on the power and versatility of generating functions to derive many of the present results. We also present the derivations in great detail because they are rather involved, and although the same results may be arrived at by alternate approaches, the formulas will tend to be much more cumbersome and less computationally efficient than the ones obtained by the generating-function methods outlined here. Because of the lengthy and detailed derivations involved, many of the intermediary results have been placed in the appendices. These intermediary results are important in their own right, as they provide useful properties of harmonic-oscillator functions in a cylindrical basis, and the mapping between cylindrical and Cartesian harmonic-oscillator bases.

In section 2, the basic formalism for the calculation of both radial and axial components of the Gaussian matrix elements by the separation method are derived. In section 3, the accuracy of the method is examined both relative to direct numerical integration, and as a function of the number of shells in the oscillator basis. The execution times for the separation method are also compared to those of the numerical integration. The mapping between harmonic-oscillator function in polar and Cartesian coordinates, needed in the development of the separation-method formalism, is derived in appendix A. In appendix B, the Gaussian two-body potential, $V(\vec{r}_1, \vec{r}_2)$, is written in separated form with respect to $\vec{r}_1$ and $\vec{r}_2$. Formulas reducing the products of harmonic-oscillator functions are derived in appendix C, and provide a powerful tool in the evaluation of integrals involving those functions. In appendix D, the result quoted in [9] for the separation-method formalism in the case of large oscillator-shell numbers is derived in detail. Finally, in appendix E, we obtain a series expansion for the direct angular integral of the Gaussian potential, which we use in the numerical integration of the potential in section 3.

2 Theory

2.1 General formalism

We wish to calculate matrix elements of the two-body potential function

$$V(\vec{r}_1, \vec{r}_2) = e^{-(\vec{r}_1 - \vec{r}_2)^2/\mu^2} \tag{2}$$

in the cylindrical harmonic-oscillator basis. We will write the matrix elements as

$$\begin{aligned} V_{ijkl} \equiv & \langle ij \,| V |\, kl \rangle \\ & = \int d^3 r_1 \int d^3 r_2 \Phi^*_{n_r^{(i)}, \Lambda^{(i)}, n_z^{(i)}}(\vec{r}_1; b_\perp, b_z)\, \Phi^*_{n_r^{(j)}, \Lambda^{(j)}, n_z^{(j)}}(\vec{r}_2; b_\perp, b_z) \\ & \quad \times V(\vec{r}_1, \vec{r}_2)\, \Phi_{n_r^{(k)}, \Lambda^{(k)}, n_z^{(k)}}(\vec{r}_1; b_\perp, b_z)\, \Phi_{n_r^{(l)}, \Lambda^{(l)}, n_z^{(l)}}(\vec{r}_2; b_\perp, b_z) \end{aligned} \tag{3}$$

where we have introduced the stretched harmonic-oscillator basis functions in the cylindrical coordinates (ρ, φ, z) [1]

$$\begin{aligned} \Phi_{n_r, \Lambda, n_z}(\vec{r}; b_\perp, b_z) &= \Phi_{n_r, \Lambda}(\rho, \varphi; b_\perp)\, \Phi_{n_z}(z; b_z) \\ &= \Phi_{n_r, |\Lambda|}(\rho; b_\perp)\, \frac{e^{\mathrm{i}\Lambda\varphi}}{\sqrt{2\pi}} \Phi_{n_z}(z; b_z) \end{aligned} \tag{4}$$

with the radial-component function

$$\Phi_{n_r, |\Lambda|}(\rho; b_\perp) = \mathcal{N}^{|\Lambda|}_{n_r} \eta^{|\Lambda|/2} e^{-\eta/2} L^{|\Lambda|}_{n_r}(\eta) \tag{5}$$

defined in terms of associated Laguerre polynomials $L^{|\Lambda|}_{n_r}(\eta)$ as a function of

$$\eta \equiv \rho^2 / b_\perp^2$$

and with a normalization constant given by

$$\mathcal{N}_{n_r, |\Lambda|} \equiv \frac{1}{b_\perp} \left[\frac{2 n_r!}{(n_r + |\Lambda|)!} \right]^{1/2} \tag{6}$$

The Cartesian, z-axis-component function in Eq. (4),

[1] We will drop the qualifier “stretched” when referring to the deformed harmonic-oscillator function in subsequent discussion for the sake of brevity.

$$\Phi_{n_z}(z;b_z) = \mathcal{N}_{n_z} e^{-\xi^2/2} H_{n_z}(\xi) \tag{7}$$

is expressed in terms of Hermite polynomials $H_{n_z}(\xi)$ with

$$\xi \equiv z/b_z$$

and normalization constant

$$\mathcal{N}_{n_z} \equiv \frac{1}{\left(b_z\sqrt{\pi}2^{n_z}n_z!\right)^{1/2}}$$

The harmonic-oscillator functions defined in Eqs. (4) and (7) satisfy the orthonormalization conditions

$$\int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi\, \Phi^*_{n_r,\Lambda}(\rho,\varphi;b_\perp)\, \Phi_{n'_r,\Lambda'}(\rho,\varphi;b_\perp) = \delta_{n_r,n'_r}\delta_{\Lambda,\Lambda'}$$

$$\int_{-\infty}^\infty dz\, \Phi_{n_z}(z;b_z)\, \Phi_{n'_z}(z;b_z) = \delta_{n_z,n'_z}$$

The parameters $b_\perp$ and b_z appearing in the harmonic-oscillator function definitions are usually treated as variational parameters in HFB calculations, and chosen to minimize the energy.

The central idea in this paper is to express the two-body potential as a sum of products of one-body potential functions

$$e^{-(\vec{r}_1-\vec{r}_2)^2/\mu^2} = \sum_{n_r,\Lambda,n_z} f_{n_r,\Lambda,n_z}(\vec{r}_1;b_\perp,b_z)\, \hat{\Phi}_{n_r,\Lambda,n_z}(\vec{r}_2;b_\perp,b_z)$$

Then the two-body matrix elements can be written in terms of one-body matrix elements

$$V_{ijkl} = \sum_{n_r,\Lambda,n_z} \langle i\left| f_{n_r,\Lambda,n_z}\right| k\rangle \left\langle j\left|\hat{\Phi}_{n_r,\Lambda,n_z}\right| l\right\rangle \tag{8}$$

where we will show that this last sum is limited to a finite number of terms. It will be useful to separate the radial and Cartesian components in each one-body matrix element to write

$$
\begin{aligned}
\langle i\left|f_{n_r,\Lambda,n_z}\right|k\rangle &= \int d^3r\, \Phi^*_{n_r^{(i)},\Lambda^{(i)},n_z^{(i)}}\left(\vec{r};b_\perp,b_z\right) f_{n_r,\Lambda,n_z}\left(\vec{r};b_\perp,b_z\right) \\
&\quad \times \Phi_{n_r^{(k)},\Lambda^{(k)},n_z^{(k)}}\left(\vec{r};b_\perp,b_z\right) \\
&= \int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi\, \Phi_{n_r^{(i)},\Lambda^{(i)}}\left(\rho,\varphi;b_\perp\right) f_{n_r,\Lambda}\left(\rho,\varphi;b_\perp\right) \\
&\quad \times \Phi_{n_r^{(k)},\Lambda^{(k)}}\left(\rho,\varphi;b_\perp\right) \\
&\quad \times \int_{-\infty}^{\infty} dz\, \Phi_{n_z^{(i)}}\left(z;b_z\right) f_{n_z}\left(z;b_z\right) \Phi_{n_z^{(k)}}\left(z;b_z\right) \\
&\equiv \langle i\left|f_{n_r,\Lambda}\right|k\rangle \langle i\left|f_{n_z}\right|k\rangle
\end{aligned}
$$

and, similarly,

$$
\begin{aligned}
\left\langle j\left|\hat{\Phi}_{n_r,\Lambda,n_z}\right|l\right\rangle &= \int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi\, \Phi_{n_r^{(j)},\Lambda^{(j)}}\left(\rho,\varphi;b_\perp\right) \hat{\Phi}_{n_r,\Lambda}\left(\rho,\varphi;b_\perp\right) \\
&\quad \times \Phi_{n_r^{(l)},\Lambda^{(l)}}\left(\rho,\varphi;b_\perp\right) \\
&\quad \times \int_{-\infty}^{\infty} dz\, \Phi_{n_z^{(j)}}\left(z;b_z\right) \hat{\Phi}_{n_z}\left(z;b_z\right) \Phi_{n_z^{(l)}}\left(z;b_z\right) \\
&\equiv \left\langle j\left|\hat{\Phi}_{n_r,\Lambda}\right|l\right\rangle \left\langle j\left|\hat{\Phi}_{n_z}\right|l\right\rangle
\end{aligned}
$$

so that we can write Eq. (8) as

$$
\begin{aligned}
V_{ijkl} &= \left[\sum_{n_r,\Lambda} \langle i\left|f_{n_r,\Lambda}\right|k\rangle \left\langle j\left|\hat{\Phi}_{n_r,\Lambda}\right|l\right\rangle\right] \left[\sum_{n_z} \langle i\left|f_{n_z}\right|k\rangle \left\langle j\left|\hat{\Phi}_{n_z}\right|l\right\rangle\right] \\
&\equiv V^{(r)}_{ijkl} V^{(z)}_{ijkl}
\end{aligned}
\tag{9}
$$

In the remainder of this section we calculate the explicit expressions needed to evaluate the matrix elements V_{ijkl}.

2.2 Cartesian component

Here we derive an expression for the Cartesian component, $V^{(z)}_{ijkl}$, in Eq. (9). We will show that

$$
V^{(z)}_{ijkl} = \sqrt{\frac{G_z-1}{G_z+1}} \sum_{m_z=\left|n_z^{(i)}-n_z^{(k)}\right|,2}^{n_z^{(i)}+n_z^{(k)}} \sum_{n_z=\left|n_z^{(j)}-n_z^{(l)}\right|,2}^{n_z^{(j)}+n_z^{(l)}} T^{m_z}_{n_z^{(i)},n_z^{(k)}} T^{n_z}_{n_z^{(j)},n_z^{(l)}} \bar{I}\left(m_z,n_z\right) \tag{10}
$$

where G_z is defined by Eq. (B.4), the $T^{n_3}_{n_1,n_2}$ coefficients by Eq. (C.6), and the $\bar{I}\left(m_z,n_z\right)$ coefficients by Eq. (18).

We start by evaluating

$$\left\langle j\left|\hat{\Phi}_{n_z}\right|l\right\rangle = \int_{-\infty}^{\infty} dz\,\Phi_{n_z^{(j)}}\left(z;b_z\right)\hat{\Phi}_{n_z}\left(z;b_z\right)\Phi_{n_z^{(l)}}\left(z;b_z\right)$$

Using Eqs. (B.1) which gives the explicit form of $\hat{\Phi}_{n_z}\left(z;b_z\right)$ and Eq. (C.1) to reduce the product of harmonic-oscillator functions,

$$\left\langle j\left|\hat{\Phi}_{n_z}\right|l\right\rangle = \frac{1}{\sqrt{b_z\sqrt{\pi}}}\sum_{m_z=\left|n_z^{(j)}-n_z^{(l)}\right|,2}^{n_z^{(j)}+n_z^{(l)}} T^{m_z}_{n_z^{(j)},n_z^{(l)}}\int_{-\infty}^{\infty} dz\,\Phi_{m_z}\left(z;b_z\right)\Phi_{n_z}\left(z;b_z\right)$$

By orthogonality of the harmonic-oscillator functions this is simply

$$\left\langle j\left|\hat{\Phi}_{n_z}\right|l\right\rangle = \frac{1}{\sqrt{b_z\sqrt{\pi}}}T^{n_z}_{n_z^{(j)},n_z^{(l)}} \tag{11}$$

where we must have $\left|n_z^{(j)}-n_z^{(l)}\right| \leq n_z \leq n_z^{(j)}+n_z^{(l)}$ for the $T^{n_z}_{n_z^{(j)},n_z^{(l)}}$ coefficient to be non-zero. Next, we use the explicit form of $f_{n_z}\left(z;b_z\right)$ from Eq. (B.2) to write

$$\begin{aligned}\left\langle i\left|f_{n_z}\right|k\right\rangle &= \int_{-\infty}^{\infty} dz\,\Phi_{n_z^{(i)}}\left(z;b_z\right)f_{n_z}\left(z;b_z\right)\Phi_{n_z^{(k)}}\left(z;b_z\right)\\ &= K_z^{1/2}\lambda_{n_z}\int_{-\infty}^{\infty} dz\,\Phi_{n_z^{(i)}}\left(z;b_z\right)e^{-z^2/\left(2G_zb_z^2\right)}\\ &\quad\times\Phi_{n_z}\left(z;G_z^{1/2}b_z\right)\Phi_{n_z^{(k)}}\left(z;b_z\right)\end{aligned} \tag{12}$$

Two of the harmonic-oscillator functions can be replaced with a single one, thanks to Eq. (C.1),

$$\begin{aligned}\left\langle i\left|f_{n_z}\right|k\right\rangle &= \frac{K_z^{1/2}\lambda_{n_z}}{\sqrt{b_z\sqrt{\pi}}}\sum_{m_z=\left|n_z^{(i)}-n_z^{(k)}\right|,2}^{n_z^{(i)}+n_z^{(k)}} T^{m_z}_{n_z^{(i)},n_z^{(k)}}\int_{-\infty}^{\infty} dz\,e^{-z^2/\left(2b_z^2\right)-z^2/\left(2G_zb_z^2\right)}\\ &\quad\times\Phi_{m_z}\left(z;b_z\right)\Phi_{n_z}\left(z;G_z^{1/2}b_z\right)\end{aligned} \tag{13}$$

The remaining integral, which we write in terms of the function

$$I\left(m,n\right) \equiv \int_{-\infty}^{\infty} dz\,e^{-z^2/\left(2b_z^2\right)-z^2/\left(2B_z^2\right)}\Phi_m\left(z;b_z\right)\Phi_n\left(z;B_z\right)$$

where $B_z \equiv G_z^{1/2}b_z$, can be calculated with the help of generating functions. Indeed, using Eq. (A.1) to form the product of the harmonic-oscillator functions, we have for any t_1 and t_2

$$e^{-t_1^2+2t_1z/b_z-z^2/\left(2b_z^2\right)}e^{-t_2^2+2t_2z/B_z-z^2/\left(2B_z^2\right)} = \sqrt{b_zB_z\pi}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{2^{(m+n)/2}}{\sqrt{m!n!}} \times t_1^m t_2^n \Phi_m\left(z;b_z\right)\Phi_n\left(z;B_z\right)$$

from which, multiplying by the Gaussian factors in the definition of $I\left(m,n\right)$ and integrating both sides of the equation,

$$e^{-t_1^2-t_2^2}\int_{-\infty}^{\infty}dz\, e^{2t_1z/b_z-z^2/b_z^2+2t_2z/B_z-z^2/B_z^2} = \sqrt{b_zB_z\pi}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{2^{(m+n)/2}}{\sqrt{m!n!}}t_1^m t_2^n I\left(m,n\right) \tag{14}$$

The integral on the left-hand side can be evaluated by completing the square,

$$\int_{-\infty}^{\infty}dz\, e^{2t_1z/b_z-z^2/b_z^2+2t_2z/B_z-z^2/B_z^2} = e^{t^2/\nu}\int_{-\infty}^{\infty}dz\, e^{-\left(\sqrt{\nu}z-t/\sqrt{\nu}\right)^2} = \sqrt{\frac{\pi}{\nu}}e^{t^2/\nu}$$

where we have defined

$$\nu \equiv \frac{1}{b_z^2}+\frac{1}{B_z^2}$$
$$t \equiv \frac{t_1}{b_z}+\frac{t_2}{B_z}$$

Thus, the left-hand side of Eq. (14) becomes

$$LHS = \sqrt{\frac{\pi}{\nu}}e^{t^2/\nu-t_1^2-t_2^2} = \sqrt{\frac{\pi}{\nu}}e^{-\left(b_zt_1-B_zt_2\right)^2/\left(\nu b_z^2B_z^2\right)}$$

which can be expanded as

$$LHS = \sqrt{\frac{\pi}{\nu}}\sum_{p=0}^{\infty}\frac{(-1)^p\left(b_zt_1-B_zt_2\right)^{2p}}{p!\left(\nu b_z^2B_z^2\right)^p} = \sqrt{\frac{\pi}{\nu}}\sum_{p=0}^{\infty}\sum_{q=0}^{2p}\begin{pmatrix}2p\\ q\end{pmatrix}\frac{(-1)^{p+q}}{p!\nu^p b_z^q B_z^{2p-q}}t_1^{2p-q}t_2^q$$

Comparing with the right-hand side of Eq. (14), we see that we must make the identifications $m=2p-q$ and $n=q$ in order for the equation to hold for any t_1 and t_2. Then,

$$LHS = \sqrt{\frac{\pi}{\nu}} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \begin{pmatrix} 2p \\ q \end{pmatrix} \frac{(-1)^{p+q}}{p! \nu^p b_z^q B_z^{2p-q}} t_1^{2p-q} t_2^q \delta_{n,q} \delta_{m,2p-q}$$

and the comparison with the right-hand side of Eq. (14) yields

$$I(m,n) = \frac{(-1)^{(m+n)/2+n} \sqrt{m!n!}}{\left(\frac{m+n}{2}\right)! (2\nu)^{(m+n)/2} b_z^n B_z^m \sqrt{b_z B_z \nu}} \begin{pmatrix} m+n \\ n \end{pmatrix}$$

Note that $m+n$ must be even. We simplify this form further by noting that

$$b_z B_z \nu = G_z^{1/2} + G_z^{-1/2} \tag{15}$$
$$B_z^2 \nu = 1 + G_z \tag{16}$$
$$b_z^2 \nu = 1 + G_z^{-1} \tag{17}$$

where G_z is defined in Eq. (B.4). This leads us to write

$$I(m,n) = \frac{G_z^{1/4} G_z^{n/2}}{\sqrt{1+G_z}} \sqrt{\frac{m!n!}{2^{m+n}}} \frac{(-1)^{(m-n)/2}}{\left(\frac{m+n}{2}\right)! (1+G_z)^{(m+n)/2}} \begin{pmatrix} m+n \\ n \end{pmatrix}$$

Some of the constants can be factored out by defining the coefficient

$$\begin{aligned} \bar{I}(m,n) &\equiv \frac{\sqrt{1+G_z}}{G_z^{1/4} G_z^{n/2}} I(m,n) \\ &= \sqrt{\frac{m!n!}{2^{m+n}}} \frac{(-1)^{(m-n)/2}}{\left(\frac{m+n}{2}\right)! (1+G_z)^{(m+n)/2}} \begin{pmatrix} m+n \\ n \end{pmatrix} \end{aligned} \tag{18}$$

Then, returning to Eq. (13), we obtain after some simplification

$$\langle i | f_{n_z} | k \rangle = \frac{K_z^{1/2} \lambda_{n_z}}{\sqrt{b_z \sqrt{\pi}}} \frac{G_z^{1/4} G_z^{n_z/2}}{\sqrt{1+G_z}} \sum_{m_z = \left| n_z^{(i)} - n_z^{(k)} \right|, 2}^{n_z^{(i)} + n_z^{(k)}} T^{m_z}_{n_z^{(i)}, n_z^{(k)}} \bar{I}(m_z, n_z) \tag{19}$$

Having derived the explicit forms in Eqs. (11) and (19), we can express the Cartesian component in Eq. (9) as

$$V_{ijkl}^{(z)} \equiv \sum_{n_z} \langle i \left| f_{n_z} \right| k \rangle \left\langle j \left| \hat{\Phi}_{n_z} \right| l \right\rangle$$
$$= \sqrt{\frac{G_z - 1}{G_z + 1}} \sum_{m_z=\left|n_z^{(i)}-n_z^{(k)}\right|,2}^{n_z^{(i)}+n_z^{(k)}} \sum_{n_z=\left|n_z^{(j)}-n_z^{(l)}\right|,2}^{n_z^{(j)}+n_z^{(l)}} T^{m_z}_{n_z^{(i)},n_z^{(k)}} T^{n_z}_{n_z^{(j)},n_z^{(l)}} \bar{I}\left(m_z, n_z\right)$$

where $\bar{I}\left(m_z, n_z\right)$ is given by Eq. (18), and the T coefficients are given by Eq. (C.6). An alternate form of $V_{ijkl}^{(z)}$ was proposed by Egido et al. [9] which yields more accurate results for large oscillator shell numbers, and is derived as Eq. (D.2) in appendix D.

2.3 Radial component

A formula similar to Eq. (10) can be derived for the radial component, $V_{ijkl}^{(r)}$, in Eq. (9). We will show that

$$V_{ijkl}^{(r)} = \frac{G_\perp - 1}{G_\perp + 1} \sum_{n_r=0}^{n_{\bar{j},l}} \sum_{n=0}^{n_{\bar{i},k}} T^{n,-\Lambda^{(i)}+\Lambda^{(k)}}_{n_r^{(i)},-\Lambda^{(i)};n_r^{(k)},\Lambda^{(k)}} T^{n_r,-\Lambda^{(j)}+\Lambda^{(l)}}_{n_r^{(j)},-\Lambda^{(j)};n_r^{(l)},\Lambda^{(l)}}$$
$$\times \bar{I}\left(n_r, -\Lambda^{(j)} + \Lambda^{(l)}; n, -\Lambda^{(i)} + \Lambda^{(k)}\right) \tag{20}$$

where $G_\perp$ is defined by Eq. (B.10), the T coefficients by Eq. (C.9), and the $\bar{I}$ coefficients by Eq. (27). The indices $n_{\bar{j},l}$ and $n_{\bar{i},k}$ are given by Eq. (A.29), where the bar indicates that $-\Lambda^{(j)}$ and $-\Lambda^{(i)}$, respectively, should be used in that definition due to the complex conjugation in Eq. (3).

Using Eqs. (B.7) for the explicit form of $\hat{\Phi}_{n_r,\Lambda}\left(\rho, \varphi; b_\perp\right)$, Eq. (C.7) to reduce the product of harmonic-oscillator functions, and the orthogonality of harmonic-oscillator functions

$$\left\langle j \left| \hat{\Phi}_{n_r,\Lambda} \right| l \right\rangle = \int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi \, \Phi^*_{n_r^{(j)},\Lambda^{(j)}}\left(\rho, \varphi; b_\perp\right) \hat{\Phi}_{n_r,\Lambda}\left(\rho, \varphi; b_\perp\right)$$
$$\times \Phi_{n_r^{(l)},\Lambda^{(l)}}\left(\rho, \varphi; b_\perp\right)$$
$$= \frac{1}{\sqrt{\pi} b_\perp} \sum_{n=0}^{n_{\bar{j},l}} T^{n,-\Lambda^{(j)}+\Lambda^{(l)}}_{n_r^{(j)},-\Lambda^{(j)};n_r^{(l)},\Lambda^{(l)}}$$
$$\times \int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi \, \Phi^*_{n,\Lambda^{(j)}+\Lambda^{(l)}}\left(\rho, \varphi; b_\perp\right) \Phi_{n_r,\Lambda}\left(\rho, \varphi; b_\perp\right)$$
$$= \frac{1}{\sqrt{\pi} b_\perp} T^{n_r,-\Lambda^{(j)}+\Lambda^{(l)}}_{n_r^{(j)},-\Lambda^{(j)};n_r^{(l)},\Lambda^{(l)}} \delta_{n_r \le n_{\bar{j},l}} \delta_{\Lambda,-\Lambda^{(j)}+\Lambda^{(l)}}$$

where the bar superscript in the $n_{\bar{j},l}$ symbol serves as a reminder that we must use $-\Lambda^{(j)}$ in Eq. (A.29), because of the complex conjugation. The condition

$\delta_{n_r \le n_{\bar{j},l}}$ comes about from the definition of the T coefficients in Eq. (C.9). The other matrix element in the radial component of Eq. (9) is written explicitly using the explicit form for $f_{n_r,\Lambda}(\rho,\varphi;b_\perp)$ in Eq. (B.8) as

$$
\begin{aligned}
\langle i\,| f_{n_r,\Lambda}|\,k\rangle =& \int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi\, \Phi^*_{n_r^{(i)},\Lambda^{(i)}}(\rho,\varphi;b_\perp)\, f_{n_r,\Lambda}(\rho,\varphi;b_\perp) \\
&\times \Phi_{n_r^{(k)},\Lambda^{(k)}}(\rho,\varphi;b_\perp) \\
=& K_\perp \lambda_{2n_r+|\Lambda|} \int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi\, e^{-\rho^2/\left(2G_\perp b_\perp^2\right)} \Phi_{n_r,\Lambda}\left(\rho,\varphi;G_\perp^{1/2} b_\perp\right) \\
&\times \Phi^*_{n_r^{(i)},\Lambda^{(i)}}(\rho,\varphi;b_\perp)\, \Phi_{n_r^{(k)},\Lambda^{(k)}}(\rho,\varphi;b_\perp)
\end{aligned}
$$

and using Eq. (C.7), the product of harmonic-oscillator functions can be reduced

$$
\begin{aligned}
\langle i\,| f_{n_r,\Lambda}|\,k\rangle =& \frac{K_\perp \lambda_{2n_r+|\Lambda|}}{\sqrt{\pi} b_\perp} \sum_{n=0}^{n_{\bar{i},k}} T^{n,-\Lambda^{(i)}+\Lambda^{(k)}}_{n_r^{(i)},-\Lambda^{(i)};n_r^{(k)},\Lambda^{(k)}} \\
&\times \int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi\, e^{-\rho^2/\left(2B_\perp^2\right)-\rho^2/\left(2b_\perp^2\right)} \\
&\times \Phi_{n_r,\Lambda}(\rho,\varphi;B_\perp)\, \Phi_{n,-\Lambda^{(i)}+\Lambda^{(k)}}(\rho,\varphi;b_\perp)
\end{aligned}
$$

where $B_\perp \equiv G_\perp^{1/2} b_\perp$, and the $\bar{i}$ in $n_{\bar{i},k}$ is a reminder that we must use $-\Lambda^{(i)}$ in Eq. (A.29). The remaining integral to be calculated is

$$
\begin{aligned}
I(n_1,k_1;n_2,k_2) \equiv& \int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi\, e^{-\rho^2/\left(2B_\perp^2\right)-\rho^2/\left(2b_\perp^2\right)} \\
&\times \Phi_{n_1,k_1}(\rho,\varphi;B_\perp)\, \Phi_{n_2,k_2}(\rho,\varphi;b_\perp)
\end{aligned} \tag{21}
$$

and can be evaluated using the generating function in Eq. (A.3) by writing, for arbitrary vectors $\vec{t}_1$ and $\vec{t}_2$,

$$
\begin{aligned}
& e^{-\vec{t}_1^2+2\vec{\rho}\cdot\vec{t}_1/B_\perp-\rho^2/\left(2B_\perp^2\right)} e^{-\vec{t}_2^2+2\vec{\rho}\cdot\vec{t}_2/b_\perp-\rho^2/\left(2b_\perp^2\right)} \\
&= B_\perp^2 \sqrt{\frac{\pi}{2}} \sum_{k_1=-\infty}^{\infty} \sum_{n_1=0}^{\infty} \mathcal{N}_{n_1,|k_1|}(B_\perp)\, \chi_{n_1,k_1}\left(\vec{t}_1\right) \Phi_{n_1,k_1}(\rho,\varphi;B_\perp) \\
&\times b_\perp^2 \sqrt{\frac{\pi}{2}} \sum_{k_2=-\infty}^{\infty} \sum_{n_2=0}^{\infty} \mathcal{N}_{n_2,|k_2|}(b_\perp)\, \chi_{n_2,k_2}\left(\vec{t}_2\right) \Phi_{n_2,k_2}(\rho,\varphi;b_\perp)
\end{aligned} \tag{22}
$$

note that, for clarity, we have explicitly written the parameter dependence for the normalization coefficients $\mathcal{N}_{n_1,|k_1|}(B_\perp)$ and $\mathcal{N}_{n_2,|k_2|}(b_\perp)$ given by Eq. (6). Multiplying both sides of Eq. (22) by the Gaussian factor that appears in Eq. (21) and integrating, we obtain on the left-hand side

$$LHS = e^{-\vec{t}_1^2-\vec{t}_2^2}\int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi\, e^{-\rho^2/B_\perp^2-\rho^2/b_\perp^2}e^{2\vec{\rho}\cdot\vec{t}_1/B_\perp}e^{2\vec{\rho}\cdot\vec{t}_2/b_\perp} \tag{23}$$

and on the right-hand side

$$\begin{aligned} RHS = & \frac{\pi}{2}B_\perp^2 b_\perp^2 \sum_{k_1=-\infty}^{\infty}\sum_{n_1=0}^{\infty}\sum_{k_2=-\infty}^{\infty}\sum_{n_2=0}^{\infty}\mathcal{N}_{n_1,|k_1|}\left(B_\perp\right)\mathcal{N}_{n_2,|k_2|}\left(b_\perp\right) \\ & \times\chi_{n_1,k_1}\left(\vec{t}_1\right)\chi_{n_2,k_2}\left(\vec{t}_2\right) I\left(n_1,k_1;n_2,k_2\right) \end{aligned} \tag{24}$$

which contains the desired coefficients $I\left(n_1,k_1;n_2,k_2\right)$. The integral in Eq. (23) can be evaluated by introducing

$$\begin{aligned} \vec{t} &\equiv \frac{\vec{t}_1}{B_\perp}+\frac{\vec{t}_2}{b_\perp} \\ \nu &\equiv \frac{1}{B_\perp^2}+\frac{1}{b_\perp^2} \end{aligned}$$

and completing the square,

$$\begin{aligned} LHS &= e^{t^2/\nu-t_1^2-t_2^2}\int_0^\infty \rho d\rho\int_0^{2\pi} d\varphi\, \exp\left[-\left(\sqrt{\nu}\vec{\rho}-\frac{\vec{t}}{\sqrt{\nu}}\right)^2\right] \\ &= \frac{\pi}{\nu}e^{t^2/\nu-t_1^2-t_2^2} \\ &= \frac{\pi}{\nu}e^{\left(2b_\perp B_\perp\vec{t}_1\cdot\vec{t}_2-B_\perp^2t_1^2-b_\perp^2t_2^2\right)/\left(B_\perp^2b_\perp^2\nu\right)} \end{aligned}$$

using Eq. (A.27) with $\vec{t}_1 \to \vec{t}_1/\left(b_\perp\sqrt{\nu}\right)$ and $\vec{t}_2 \to \vec{t}_2/\left(B_\perp\sqrt{\nu}\right)$, this can be further expanded as

$$\begin{aligned} LHS = & \frac{\pi B_\perp^2 b_\perp^2}{2}e^{-\left(B_\perp^2t_1^2+b_\perp^2t_2^2\right)/\left(B_\perp^2b_\perp^2\nu\right)}\sum_{n=0}^{\infty}\sum_{k=-\infty}^{\infty}\mathcal{N}_{n,|k|}^2\left(B_\perp b_\perp\sqrt{\nu}\right) \\ & \times\chi_{n,k}^*\left(\frac{\vec{t}_1}{b_\perp\sqrt{\nu}}\right)\chi_{n,k}\left(\frac{\vec{t}_2}{B_\perp\sqrt{\nu}}\right) \end{aligned}$$

Next, we use Eq. (A.23) to eliminate the remaining exponential,

$$\begin{aligned} LHS = & \frac{\pi B_\perp^2 b_\perp^2}{2}\sum_{n=0}^{\infty}\sum_{k=-\infty}^{\infty}\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\frac{\left(n+m_1\right)!\left(n+m_2\right)!}{m_1!m_2!\left(n!\right)^2}\mathcal{N}_{n,|k|}^2\left(B_\perp b_\perp\sqrt{\nu}\right) \\ & \times\chi_{n+m_1,k}^*\left(\frac{\vec{t}_1}{b_\perp\sqrt{\nu}}\right)\chi_{n+m_2,k}\left(\frac{\vec{t}_2}{B_\perp\sqrt{\nu}}\right) \end{aligned}$$

Using Eqs (A.24) to eliminate the complex conjugation, and (A.25) to factor out the coefficients inside the χ functions, this takes the form

$$
\begin{aligned}
LHS = & \frac{\pi B_\perp^2 b_\perp^2}{2} \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(n+m_1)!\,(n+m_2)!}{m_1! m_2!\,(n!)^2} \mathcal{N}_{n,|k|}^2 \left(B_\perp b_\perp \sqrt{\nu}\right) \\
& \times \left(b_\perp \sqrt{\nu}\right)^{-2(n+m_1)-|k|} \left(B_\perp \sqrt{\nu}\right)^{-2(n+m_2)-|k|} \\
& \times \chi_{n+m_1,-k}\left(\vec{t}_1\right) \chi_{n+m_2,k}\left(\vec{t}_2\right)
\end{aligned}
$$

Comparing this result for LHS with RHS in Eq. (24) for arbitrary vectors $\vec{t}_1$ and $\vec{t}_2$, we are led to conclude that

$$
I\left(n_1, k_1; n_2, k_2\right) = 0 \quad \text{if } k_1 + k_2 \neq 0 \tag{25}
$$

We are also led to make the identifications

$$
\begin{aligned}
n + m_1 &= n_1 \\
n + m_2 &= n_2 \\
-k &= k_1 \\
k &= k_2
\end{aligned}
$$

which allow us to write

$$
\begin{aligned}
LHS = & \frac{\pi B_\perp^2 b_\perp^2}{2} \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \frac{n_1! n_2!}{(n_1-n)!\,(n_2-n)!\,(n!)^2} \mathcal{N}_{n,|k|}^2 \left(B_\perp b_\perp \sqrt{\nu}\right) \\
& \times \left(b_\perp \sqrt{\nu}\right)^{-2n_1-|k|} \left(B_\perp \sqrt{\nu}\right)^{-2n_2-|k|} \chi_{n_1,-k}\left(\vec{t}_1\right) \chi_{n_2,k}\left(\vec{t}_2\right)
\end{aligned} \tag{26}
$$

and therefore, assuming $|k_1| = |k_2| \equiv |k|$ because of Eq. (25), the comparison between LHS and RHS, in Eqs. (26) and (24) respectively, yields

$$
\begin{aligned}
I\left(n_1, k_1; n_2, k_2\right) = & \frac{\delta_{k_1+k_2,0} \left(b_\perp \sqrt{\nu}\right)^{-2n_1-|k|} \left(B_\perp \sqrt{\nu}\right)^{-2n_2-|k|} n_1! n_2!}{\mathcal{N}_{n_1,|k|}\left(B_\perp\right) \mathcal{N}_{n_2,|k|}\left(b_\perp\right)} \\
& \times \sum_{n=0}^{\infty} \frac{\mathcal{N}_{n,|k|}^2 \left(B_\perp b_\perp \sqrt{\nu}\right)}{(n_1-n)!\,(n_2-n)!\,(n!)^2} \\
= & \delta_{k_1+k_2,0} \frac{\left(b_\perp \sqrt{\nu}\right)^{-2n_1-|k|} \left(B_\perp \sqrt{\nu}\right)^{-2n_2-|k|}}{B_\perp b_\perp \nu} \\
& \times \sqrt{n_1!\,(n_1+|k|)! n_2!\,(n_2+|k|)!} \\
& \sum_{n=0}^{\infty} \frac{1}{(n_1-n)!\,(n_2-n)! n!\,(n+|k|)!}
\end{aligned}
$$

Using Eqs. (15)-(17) with $G_\perp$ instead of G_z we can simplify the factor outside the summation

$$\frac{\left(b_\perp\sqrt{\nu}\right)^{-2n_1-|k|}\left(B_\perp\sqrt{\nu}\right)^{-2n_2-|k|}}{B_\perp b_\perp \nu} = \frac{\left(1+G_\perp^{-1}\right)^{-n_1-|k|/2}\left(1+G_\perp\right)^{-n_2-|k|/2}}{G_\perp^{1/2}+G_\perp^{-1/2}}$$
$$= \frac{G_\perp^{(n_1-n_2)/2}}{\left(G_\perp^{1/2}+G_\perp^{-1/2}\right)^{n_1+n_2+|k|+1}}$$

and, for compactness of notation, we define

$$\Xi\left(n_1,n_2,|k|\right) \equiv \sum_{n=0}^{\infty} \frac{1}{\left(n_1-n\right)!\left(n_2-n\right)!n!\left(n+|k|\right)!}$$

which, after some simplification can be written as

$$\Xi\left(n_1,n_2,|k|\right) = \frac{1}{n_1!\left(n_2+|k|\right)!}\sum_{n=0}^{\infty}\begin{pmatrix} n_1 \\ n \end{pmatrix}\begin{pmatrix} n_2+|k| \\ n_2-n \end{pmatrix}$$
$$= \frac{1}{\left(n_1+n_2+|k|\right)!}\begin{pmatrix} n_1+n_2+|k| \\ n_1 \end{pmatrix}\begin{pmatrix} n_1+n_2+|k| \\ n_2 \end{pmatrix}$$

where Eq. 0.156(1) in [8] was used to obtain the second line. Therefore, we finally have

$$I\left(n_1,k_1;n_2,k_2\right) = \delta_{k_1+k_2,0}\frac{G_\perp^{(n_1-n_2)/2}}{\left(G_\perp^{1/2}+G_\perp^{-1/2}\right)^{n_1+n_2+|k|+1}}$$
$$\times\sqrt{n_1!\left(n_1+|k|\right)!n_2!\left(n_2+|k|\right)!}\,\Xi\left(n_1,n_2,|k|\right)$$

As in Eq. (18), it will be convenient to factor out some constant terms. Therefore we define

$$\bar{I}\left(n_1,k_1;n_2,k_2\right) \equiv \frac{K_\perp\lambda_{2n_1+|k|}}{\pi b_\perp^2}\frac{G_\perp+1}{G_\perp-1}I\left(n_1,k_1;n_2,k_2\right)$$
$$= \delta_{k_1+k_2,0}\frac{\sqrt{n_1!\left(n_1+|k|\right)!n_2!\left(n_2+|k|\right)!}}{\left(G_\perp+1\right)^{n_1+n_2+|k|}}\Xi\left(n_1,n_2,|k|\right) \quad (27)$$

and the radial component in Eq. (9) becomes

$$
\begin{aligned}
V_{ijkl}^{(r)} &= \sum_{n_r,\Lambda} \langle i \left| f_{n_r,\Lambda} \right| k \rangle \left\langle j \left| \hat{\Phi}_{n_r,\Lambda} \right| l \right\rangle \\
&= \frac{G_\perp - 1}{G_\perp + 1} \sum_{n_r=0}^{\infty} \sum_{\Lambda=-\infty}^{\infty} \sum_{n=0}^{n_{\bar{i},k}} T^{n,-\Lambda^{(i)}+\Lambda^{(k)}}_{n_r^{(i)},-\Lambda^{(i)};n_r^{(k)},\Lambda^{(k)}} \bar{I}\left(n_r,\Lambda;n,-\Lambda^{(i)}+\Lambda^{(k)}\right) \\
&\times T^{n_r,\Lambda^{(j)}+\Lambda^{(l)}}_{n_r^{(j)},\Lambda^{(j)};n_r^{(l)},\Lambda^{(l)}} \delta_{n_r \le n_{j,l}} \delta_{\Lambda,-\Lambda^{(j)}+\Lambda^{(l)}} \\
&= \frac{G_\perp - 1}{G_\perp + 1} \sum_{n_r=0}^{n_{\bar{j},l}} \sum_{n=0}^{n_{\bar{i},k}} T^{n,-\Lambda^{(i)}+\Lambda^{(k)}}_{n_r^{(i)},-\Lambda^{(i)};n_r^{(k)},\Lambda^{(k)}} T^{n_r,-\Lambda^{(j)}+\Lambda^{(l)}}_{n_r^{(j)},-\Lambda^{(j)};n_r^{(l)},\Lambda^{(l)}} \\
&\times \bar{I}\left(n_r,-\Lambda^{(j)}+\Lambda^{(l)};n,-\Lambda^{(i)}+\Lambda^{(k)}\right)
\end{aligned}
$$

Thus , using Eqs. (10) or (D.2) and (20), the full matrix element V_{ijkl} in Eq. (9) can be calculated as an analytical expression. In the next section, we will examine the computational merits of these results.

3 Discussion

In this section, we will compare three different ways of evaluating the Cartesian ($V_{ijkl}^{(z)}$) and radial ($V_{ijkl}^{(r)}$) components of the Gaussian matrix elements in Eq. (3): 1) direct numerical integration of Eq. (3), 2) numerical evaluation of the separation-method equations (Eqs. (10) or (D.2) for the Cartesian component, and Eq. (20) for the radial component) in double-precision mode, and 3) exact evaluation of the separation-method equations using the symbolic-algebra package Mathematica [10]. In principle, the first two methods–numerical evaluation by either integration or the separation method–will give the values of $V_{ijkl}^{(z)}$ and $V_{ijkl}^{(r)}$ to within the limits of machine accuracy and roundoff errors, whereas the third–exact evaluation of the separation-method equations using Mathematica–will produce these matrix elements to any desired accuracy (even beyond machine accuracy) and will serve as a reference check for numerical convergence of the integrals and roundoff errors.

We begin by comparing the relative merits of the separation-method Eqs. (10) and (D.2) for the Cartesian component of the matrix element. The two equations are mathematically equivalent, but Eq. (D.2) was obtained from Eq. (10) specifically to provide greater accuracy in numerical calculations. For all quantitative applications in this work, we have used

$$
\begin{aligned}
\mu &= 1.2 \text{ fm} \\
b_z &= 3.3 \text{ fm} \\
b_\perp &= 2 \text{ fm}
\end{aligned}
$$

These values of μ, b_z, $b_\perp$ are typical in HFB calculations using the Gogny interaction for ^{240}Pu along the most likely path to scission [11].

In practice, both Eqs. (10) and (D.2) can be evaluated efficiently because the $T^{n}_{n_1,n_2}$ and $\bar{I}\,(m,n)$ or $\bar{F}^{n}_{n_1,n_2}$ coefficients can easily be calculated once and for all and stored with relatively little memory, to be used in reconstructing the matrix elements $V^{(z)}_{ijkl}$ whenever they are needed. However, for large values of the quantum numbers n_i, n_j, n_k, and n_l the sums in Eq. (10) rapidly lead to sizable numerical inaccuracies. These inaccuracies arise because the T coefficients grow progressively larger with increasing values of the arguments, whereas the $\bar{I}$ coefficients decrease. The resulting sum of products of small and large numbers in Eq. (10) becomes numerically unstable. The formula obtained by Egido et al. in [9], and derived as Eq. (D.2) in the present work, avoids this problem.

Fig. 1 gives the maximum deviation between matrix elements calculated using numerical evaluations of Eqs. (10) and (D.2). To generate the plot, the equations were compared for calculations of $V^{(z)}_{ijkl}$ as a function of the maximum harmonic-oscillator shell number N_0, i.e. for all possible quantum numbers such that $0 \leq n_i, n_j, n_k, n_l \leq N_0$, and the largest deviation was recorded for each point on the plot. We will refer to N_0 as the size of the basis in the discussion below. The deviations plotted in Fig. 1 are based on the dimensionless Gaussian function in Eq. (2), but with realistic interaction strengths for the Gogny force [12], a deviation as small as 10^{-2} on the plot, can correspond to a discrepancy of the order of an MeV. Thus, for N_0 greater than about 16, Eq. (D.2) should certainly always be used instead of Eq. (10), and in the remainder of this paper we will use it consistently for all N_0 instead of Eq. (10).

Next, we compare an exact evaluation of Eq. (D.2) to the numerical integration of the Cartesian component in Eq. (3). We choose to compare the separation method to a numerical integral of the potential because the latter is easily implemented, requires very little computer memory, and can be made arbitrarily accurate. The exact evaluation of Eq. (D.2) was obtained using the symbolic-algebra package Mathematica. Within Mathematica, the expression in Eq. (D.2) was first reduced by symbolic manipulation to the exact algebraic form $a\sqrt{b}/c$, where a, b, and c are integers, for each choice of the quantum numbers n_i, n_j, n_k, and n_l. That algebraic number could then be evaluated numerically to any desired accuracy. The numerical integration, on the other hand, was performed by Gauss-Hermite quadrature in double-precision mode (i.e., with 16 significant figures). The purpose of the comparison between the exact evaluation of Eq. (D.2) and the numerical integration is to show that the numerical integration can be made arbitrarily close (up to the limits of machine accuracy) to the exact result, thereby validating Eq. (D.2). In Fig. 2, the maximum deviation between the exact calculation and numerical integration of the $V^{(z)}_{ijkl}$ values is plotted as a function of the number N_{quad} of

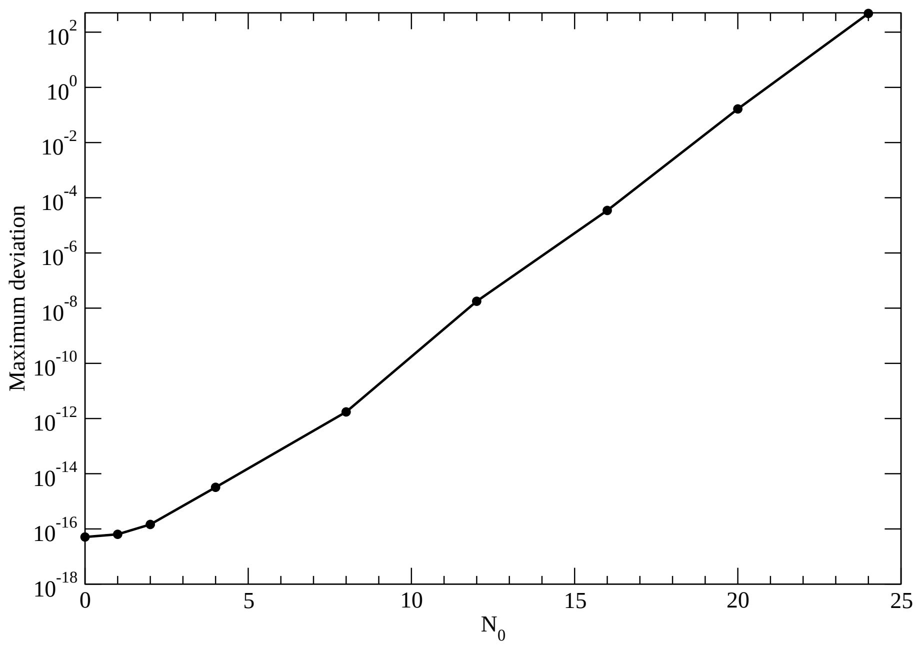

Figure 1. Maximum deviation between calculations of the matrix elements $V^{(z)}_{ijkl}$ using the separation method in Eq. (10) on one hand, and Eq. (D.2) on the other, plotted as a function of basis size N_0.

quadrature points for a basis size $N_0 = 12$. For $N_{\text{quad}} \geq 208$, the limits of machine accuracy are reached in the numerical integration, and the maximum deviation between the two methods of calculating $V^{(z)}_{ijkl}$ matrix elements levels out slightly above 4.3×10^{-16}.

In Fig. 3, we compare the exact evaluation of Eq. (D.2) using Mathematica to its numerical evaluation in double-precision mode, as a function of basis size N_0. The trend in Fig. 3 shows the effect of roundoff error in the numerical evaluation of Eq. (D.2). However, despite a clear decrease in accuracy with increasing basis size, Fig. 3 shows that a double-precision numerical evaluation of Eq. (D.2) still gives the value of the matrix elements $V^{(z)}_{ijkl}$ to a very high level of accuracy. Even for a basis size as large as $N_0 = 24$, the largest deviation from the exact values is still only 1.5×10^{-8}. For the remainder of this discussion, we will use the numerical evaluation of Eq. (D.2) in double-precision mode rather than the exact Mathematica result, because the Mathematica calculations are prohibitively time-consuming, and the accuracy of the numerical evaluation of the separation-method formulas is more than sufficient for most applications.

In Fig. 4, we extract the number of Gauss-Hermite quadrature points required by the numerical integration to obtain values that are satisfactorily close (say,

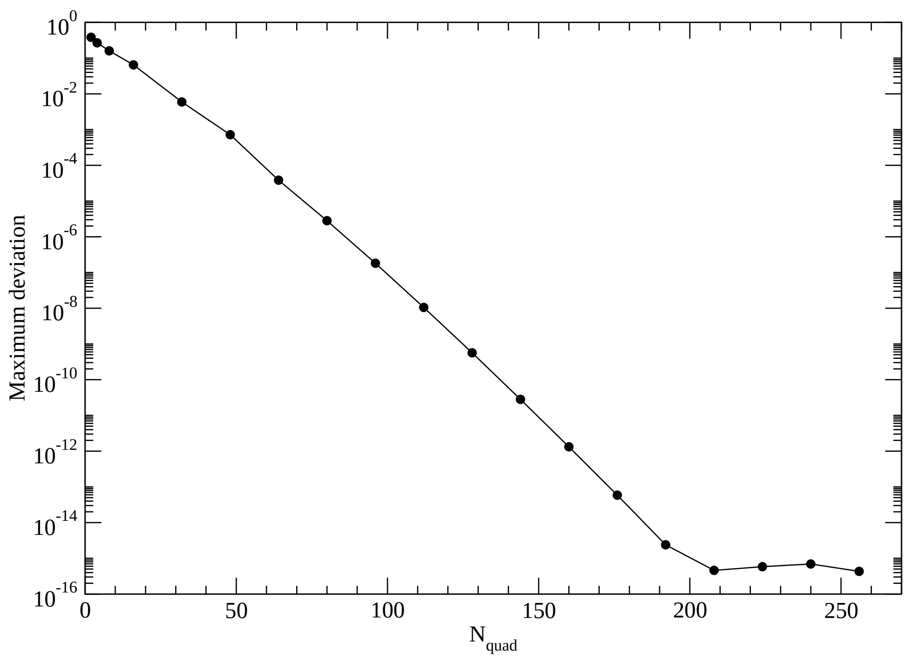

Figure 2. Maximum deviation between the numerical integration of the matrix elements $V^{(z)}_{ijkl}$ and their exact evaluation using the separation method in Eq. (D.2) with Mathematica for basis size $N_0 = 12$, plotted as a function of the number of Gauss-Hermite quadrature points in the integral.

within a 10^{-4} discrepancy at most) to the values given by a numerical evaluation of Eq. (D.2). The number of quadrature points plotted as a function of basis size N_0 is moderately large, and increases steadily with N_0. Further below we will gauge the cost in computational time incurred by the numerical integration with these relatively large numbers of quadrature points.

We carry out a similar analysis for the radial component,$V^{(r)}_{ijkl}$, of the matrix elements. In this case, for a given basis size N_0, the quantum numbers for the radial matrix element $V^{(r)}_{ijkl}$ in Eq. (3) take on all values such that $0 \leq 2n_r + |\Lambda| \leq N_0$ with $n_r \geq 0$. As we did in Fig. 2 for the Cartesian component, we compare in Fig. 5 an exact (Mathematica) calculation of Eq. (20) to a numerical integration of the radial component in Eq. (3) using double-precision Gauss-Laguerre quadrature, for a basis size $N_0 = 8$. In Fig. 5, the maximum deviation between exact evaluation and numerical integration, plotted as a function of the number N_{quad} of quadrature points, is made arbitrarily small with increasing N_{quad} values until the limits of machine accuracy and roundoff error are reached for $N_{\text{quad}} \geq 48$, where the maximum discrepancy settles above 1.3×10^{-15}.

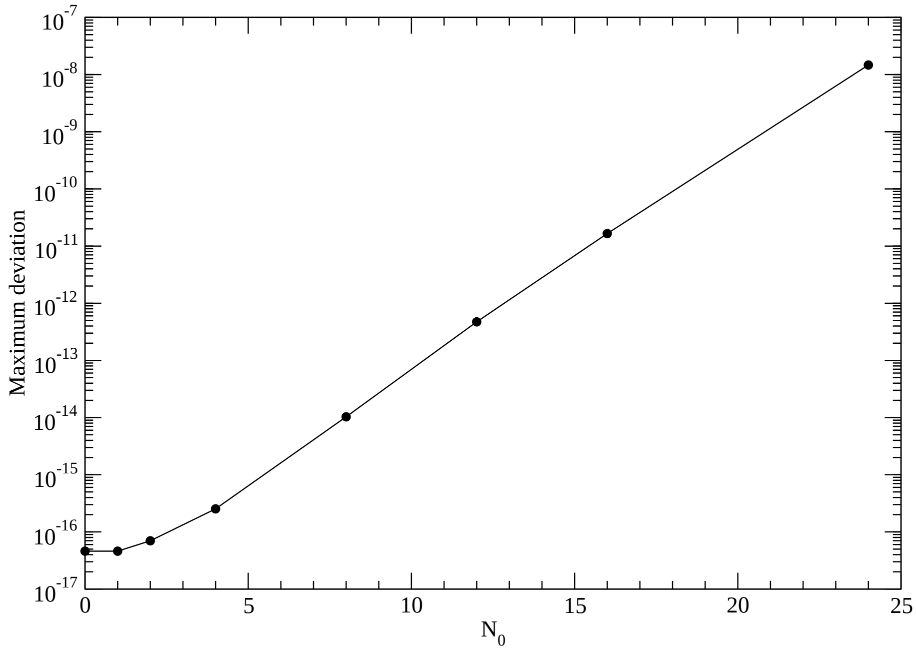

Figure 3. Maximum deviation between the numerical calculation and exact Mathematica evaluation of the matrix elements $V^{(z)}_{ijkl}$ using the separation method in Eq. (D.2), plotted as a function of basis size N_0.

A comparison between exact (Mathematica) and double-precision numerical evaluations of the separation-method result in Eq. (20) is plotted in Fig. 6 as a function of basis size N_0. The accuracy of the numerical evaluation clearly deteriorates with increasing basis size, but remains quite good nevertheless, reaching only a 1.2×10^{-9} maximum deviation for $N_0 = 12$. For practical reasons, we will use the numerical evaluation of Eq. (20) in the remainder of this discussion, rather than the exact–but much slower–Mathematica calculation.

The number of Gauss-Laguerre quadrature points needed to obtain a discrepancy of 10^{-4} or less between the numerical integration and numerical separation method for $V^{(r)}_{ijkl}$ matrix elements is plotted in Fig. 7 as a function of basis size. As in Fig. 4 for the Cartesian matrix elements, the required number of quadrature points is moderate and increases with basis size. The impact of these numbers of quadrature points on execution time will be investigated next.

We now compare execution times for the numerical integration and numerical separation methods. The numerical integrations for the Cartesian and radial components are performed with the number of quadrature points given in Figs. 4 and 7, respectively, to ensure agreement to 10^{-4} or better with the

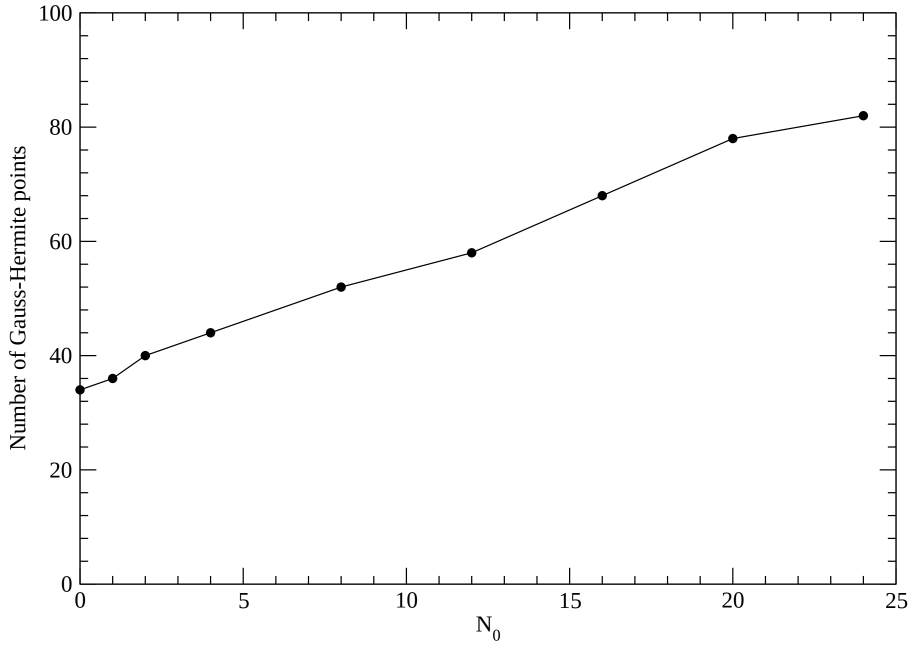

Figure 4. Minimum number of Gauss-Hermite quadrature points needed to achieve 10^{-4} or better agreement between the numerical integration of the matrix elements $V^{(z)}_{ijkl}$ and their evaluation using the separation method in Eq. (D.2), plotted as a function of basis size N_0.

separation-method results. In order to speed up the numerical integrations, the harmonic-oscillator functions are calculated at the appropriate quadrature points and stored once and for all. A set of nested loops then evaluate the multidimensional integrals by recalling the stored values of the functions as the terms in the quadrature are summed. Likewise, for the calculations by the separation method, the T, $\bar{I}$, and $\bar{F}$ coefficients are calculated ahead of time and recalled as needed in the evaluation of the matrix elements using Eqs. (D.2) and (20).

The calculations have been performed on a 2.13-GHz Pentium M processor in double-precision mode. The execution times are plotted in Fig. 8 for the z component of the matrix element, and in Fig. 9 for the radial component. The times plotted include the setup time needed to pre-calculate the harmonic-oscillator function values and separation coefficients appropriate to each method. The difference in execution times between the numerical and separation methods become staggering with increasing basis size. For large-scale computations requiring matrix-element calculations over a range of values of the harmonic-oscillator parameters $b_\perp$ and b_z, such as maps of fission shapes for a single nucleus or maps of nuclear properties for large sets of nuclei, direct

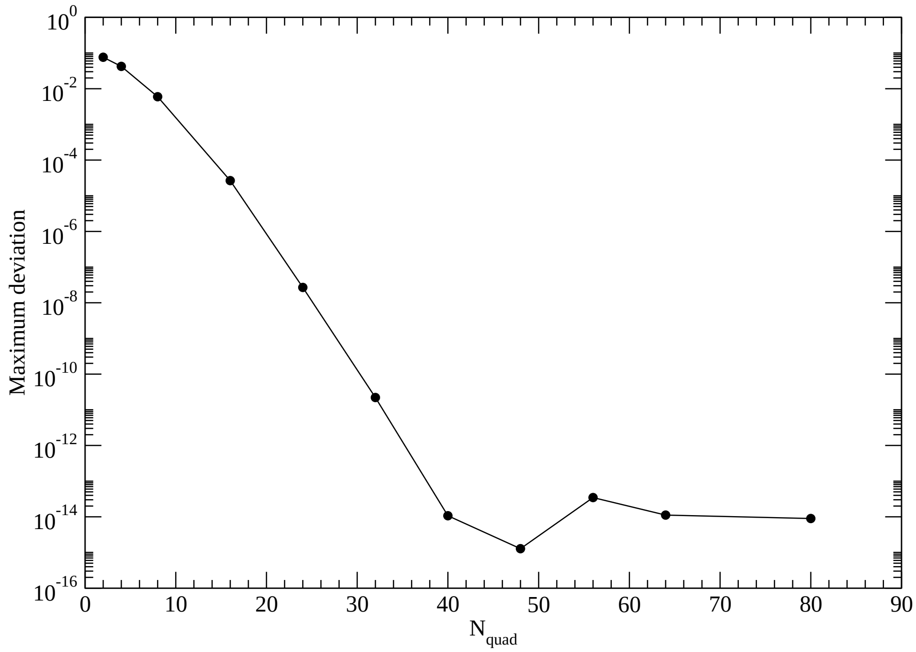

Figure 5. Maximum deviation between the numerical integration of the matrix elements $V_{ijkl}^{(r)}$ and their exact evaluation using the separation method in Eq. (20) with Mathematica for basis size $N_0 = 8$, plotted as a function of the number of Gauss-Laguerre quadrature points in the integral.

numerical integrations rapidly become unfeasible without parallel machines. Even with parallel processing, modern nuclear-physics problems (e.g., the microscopic treatment of fission in a multidimensional collective-coordinate space) will eventually overwhelm any given computational resource, and in order to match the accuracy of the separation method, numerical integrals will generally require an inordinate number of quadrature points.

4 Conclusion

We have derived explicit expressions for Gaussian matrix elements in a cylindrical harmonic-oscillator basis, using the separation method. These expressions have been tested against direct numerical integration and found to be highly accurate and computationally efficient. These characteristics make the separation method an invaluable tool for computationally-intensive applications, such as the microscopic description of fission. The work presented here has wider relevance than to the Gaussian form, or to nuclear-physics problems alone. In particular, the methodology used in the present derivations, which

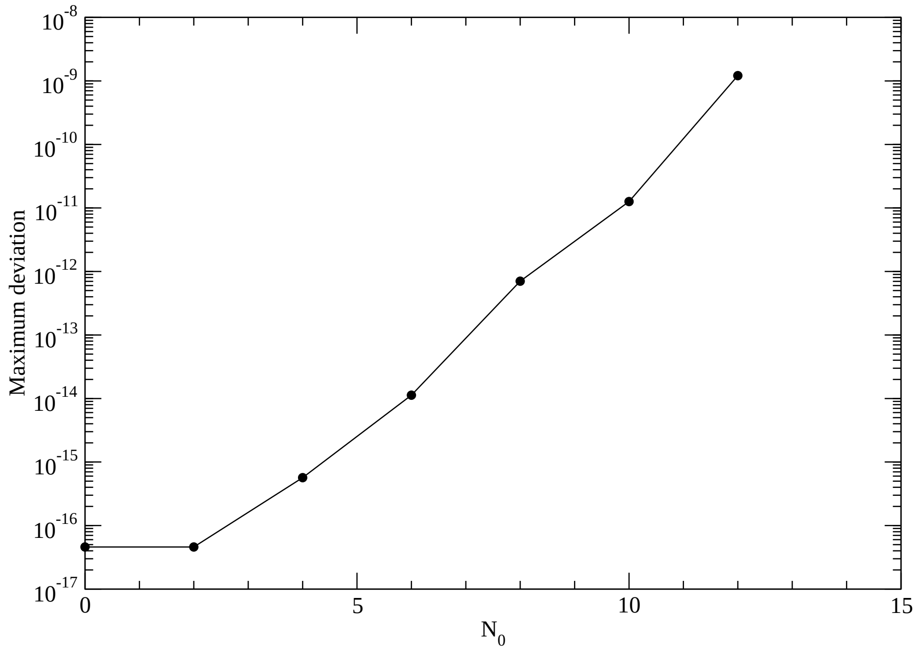

Figure 6. Maximum deviation between the numerical calculation and exact Mathematica evaluation of the matrix elements $V_{ijkl}^{(r)}$ using the separation method in Eq. (20), plotted as a function of basis size N_0.

relies heavily on generating functions, can be applied to other types of interactions and a wider class of basis states to derive analytical, computationally-efficient expressions for matrix elements. For example, in future publications, we will apply the separation method to the Coulomb and Yukawa interactions, and extend the formalism to bases of displaced and two-center deformed harmonic oscillators. These planned extensions to the separation formalism enlarge the range of applications of the method to many problems of central importance in nuclear, atomic, and molecular systems.

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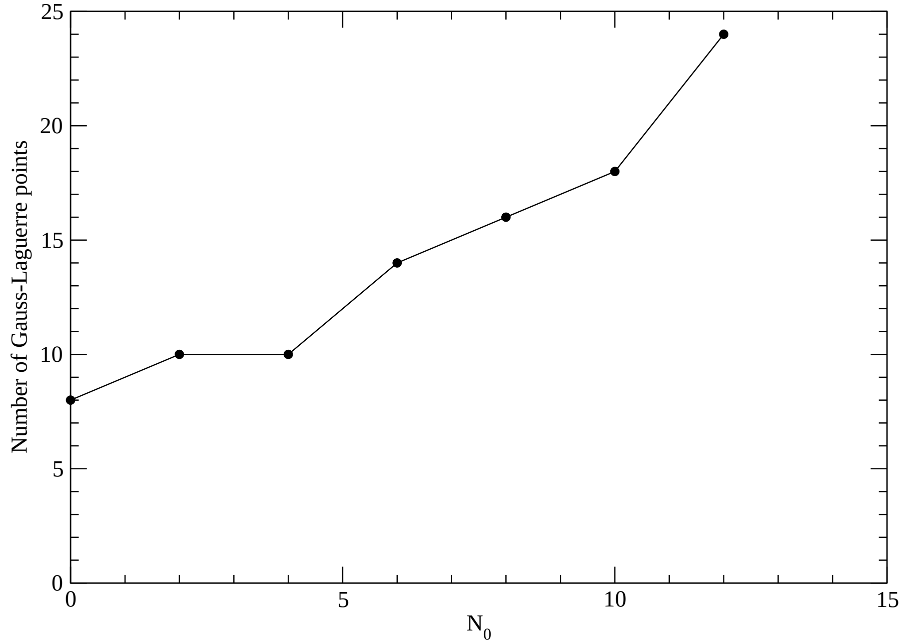

Figure 7. Minimum number of Gauss-Laguerre quadrature points needed to achieve 10^{-4} or better agreement between the numerical integration of the matrix elements $V_{ijkl}^{(r)}$ and their evaluation using the separation method in Eq. (20), plotted as a function of basis size N_0.

A Mapping between Cartesian and polar coordinates for harmonic-oscillator functions

In this section, we derive an identity relating the harmonic-oscillator functions expressed in two-dimensional Cartesian coordinates (x, y) to those in polar coordinates (ρ, φ) where

$$\begin{aligned} \rho^2 &= x^2 + y^2 \\ \tan\varphi &= \frac{y}{x} \end{aligned}$$

To this end, we will first need to derive generating functions for the harmonic-oscillator functions in the two coordinate systems.

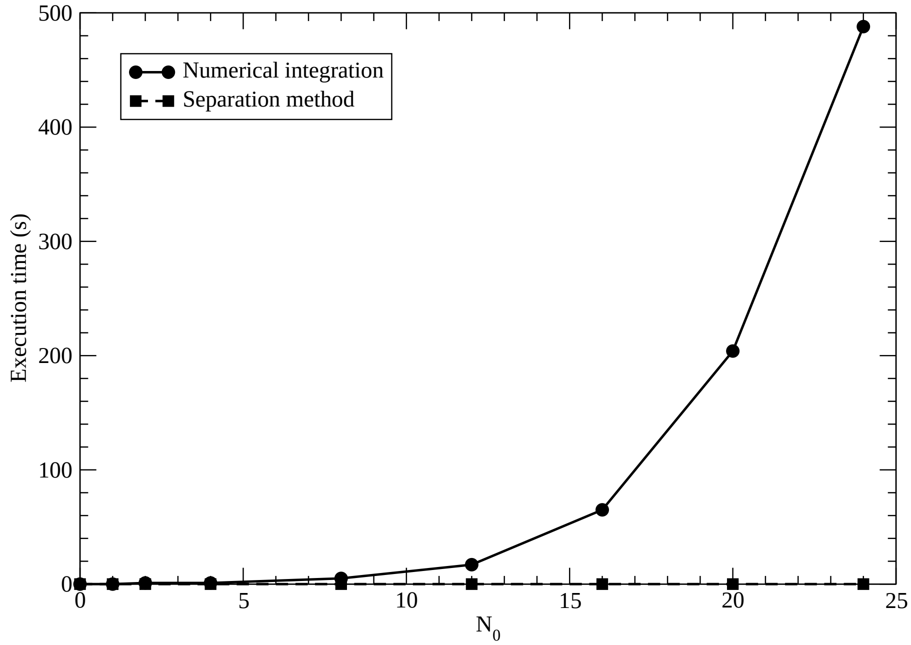

Figure 8. Comparison of total execution times for the evaluation of $V^{(z)}_{ijkl}$ by numerical integration and by the separation method in Eq. (D.2), as a function of basis size N_0.

A.1 Generating function in Cartesian coordinates

In this appendix, we derive the generating function

$$\boxed{e^{-t^2+2tx/b-x^2/\left(2b^2\right)} = \sqrt{b\sqrt{\pi}}\sum_{k=0}^{\infty}\frac{2^{k/2}}{\sqrt{k!}}t^k\Phi_k\left(x;b\right)} \tag{A.1}$$

for the Cartesian harmonic-oscillator functions in Eq. (7).

We begin with the generating function for Hermite polynomials (Eq. 8.957(1), p. 1034 in [8]), for arbitrary variables x and t,

$$e^{-t^2+2tx} = \sum_{k=0}^{\infty}\frac{t^k}{k!}H_k\left(x\right)$$

making the substitution $x \to x/b$ in order to introduce the harmonic-oscillator parameter b,

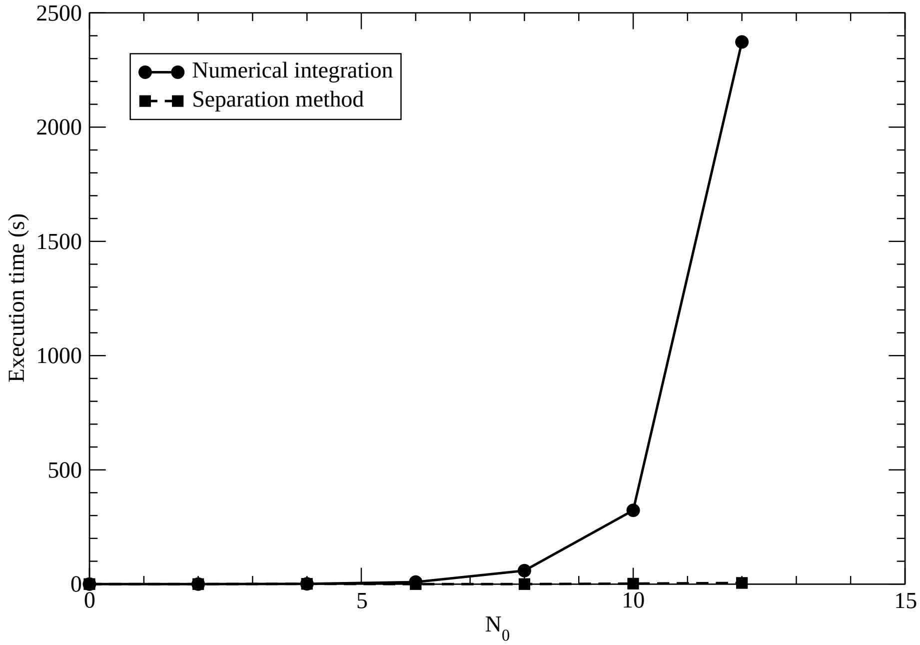

Figure 9. Comparison of total execution times for the evaluation of $V_{ijkl}^{(r)}$ by numerical integration and by the separation method in Eq. (20), as a function of basis size N_0.

$$e^{-t^2+2tx/b} = \sum_{k=0}^{\infty} \frac{t^k}{k!} H_k\left(\frac{x}{b}\right)$$

Next, we introduce the Gaussian and normalization factors appearing in the definition of the harmonic oscillator function in Eq. (7)

$$e^{-x^2/\left(2b^2\right)} e^{-t^2+2tx/b} = \sum_{k=0}^{\infty} \frac{t^k}{k!\mathcal{N}_k} \mathcal{N}_k e^{-x^2/\left(2b^2\right)} H_k\left(\frac{x}{b}\right)$$

or, in terms of the harmonic-oscillator functions,

$$e^{-t^2+2tx/b-x^2/\left(2b^2\right)} = \sqrt{b\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{2^{k/2}}{\sqrt{k!}} t^k \Phi_k\left(x;b\right)$$

A.2 Generating function in polar coordinates

Here, we derive a generating function for the polar harmonic-oscillator functions defined in Eq. (4),

$$\boxed{e^{-t^2+2\rho t\cos\varphi/b-\rho^2/\left(2b^2\right)} = b\sqrt{\pi}\sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty}\frac{(-1)^n\, t^{2n+|k|}}{\sqrt{n!\,(n+|k|)!}}\Phi_{n,k}\left(\rho,\varphi;b\right)} \tag{A.2}$$

which we also cast in the form

$$\boxed{e^{-\vec{t}^2+2\vec{\rho}\cdot\vec{t}/b-\rho^2/\left(2b^2\right)} = b^2\sqrt{\frac{\pi}{2}}\sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty}\mathcal{N}_{n,|k|}\chi_{n,k}\left(\vec{t}\right)\Phi_{n,k}\left(\rho,\varphi;b\right)} \tag{A.3}$$

where the functions $\chi_{n,k}\left(\vec{t}\right)$ are defined by Eq. (A.9).

To derive a generating function for harmonic-oscillator functions in polar coordinates, we begin with the generating function for Laguerre polynomials (Eq. 8.975(3), p. 1038 in [8]), for arbitrary variables x and z, and $\alpha > -1$

$$J_\alpha\left(2\sqrt{xz}\right)e^z\left(xz\right)^{-\alpha/2} = \sum_{n=0}^{\infty}\frac{z^n}{\Gamma\left(n+\alpha+1\right)}L_n^\alpha\left(x\right) \tag{A.4}$$

In order to match the definition of the harmonic-oscillator function in Eq. (5), we substitute $\sqrt{x} = \rho/b$, $\sqrt{z} = -it$, and $\alpha = |k|$ where k is an integer. Then, isolating the Bessel function on the left-hand side, Eq. (A.4) takes the form

$$J_{|k|}\left(-2i\rho t/b\right) = e^{t^2}\left(-i\right)^{|k|}\left(\frac{\rho t}{b}\right)^{|k|}\sum_{n=0}^{\infty}\frac{(-1)^n\, t^{2n}}{(n+|k|)!}L_n^{|k|}\left(\frac{\rho^2}{b^2}\right) \tag{A.5}$$

On the other hand, the generating function for a Bessel function of the first kind for arbitrary z and φ is (Eq. 8.511(4), p. 973 in [8])

$$\begin{aligned} e^{iz\cos\varphi} &= \sum_{k=-\infty}^{\infty} i^k J_k\left(z\right)e^{ik\varphi} \\ &= \sum_{k=-\infty}^{\infty} i^{|k|} J_{|k|}\left(z\right)e^{ik\varphi} \end{aligned} \tag{A.6}$$

where the second line follows from Eq. 8.404(2) in [8]. Substituting $z = -2i\rho t/b^2$ into Eq. (A.6),

$$e^{2\rho t\cos\varphi/b} = \sum_{k=-\infty}^{\infty} i^{|k|} J_{|k|}\left(-2i\frac{\rho t}{b}\right) e^{ik\varphi} \tag{A.7}$$

Finally, plugging Eq. (A.5) into Eq. (A.7) yields

$$\begin{aligned} e^{2\rho t\cos\varphi/b} = e^{t^2} \sum_{k=-\infty}^{\infty} (-i)^{|k|}\, i^{|k|} \left(\frac{\rho t}{b}\right)^{|k|} \\ \times \sum_{n=0}^{\infty} \frac{(-1)^n\, t^{2n}}{(n+|k|)!} L_n^{|k|}\left(\frac{\rho^2}{b^2}\right) e^{ik\varphi} \end{aligned}$$

where the right-hand side can be made to look more like the harmonic-oscillator function definition in Eq. (5),

$$\begin{aligned} e^{-t^2+2\rho t\cos\varphi/b} = \sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty} (-1)^n\, \frac{t^{2n+|k|}}{(n+|k|)!} \frac{\sqrt{2\pi} e^{\rho^2/\left(2b^2\right)}}{\mathcal{N}_{n,|k|}} \\ \times \left[\mathcal{N}_{n,|k|} \left(\frac{\rho}{b}\right)^{|k|} e^{-\rho^2/\left(2b^2\right)} L_n^{|k|}\left(\frac{\rho^2}{b^2}\right) \frac{e^{ik\varphi}}{\sqrt{2\pi}}\right] \end{aligned}$$

or, after straightforward simplifications,

$$e^{-t^2+2\rho t\cos\varphi/b-\rho^2/\left(2b^2\right)} = b\sqrt{\pi} \sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty} \frac{(-1)^n\, t^{2n+|k|}}{\sqrt{n!\,(n+|k|)!}} \Phi_{n,k}\left(\rho,\varphi;b\right)$$

Note that there is a potential ambiguity in the meaning of the angle φ in Eq. (A.2). In fact, Eq. (A.2) was derived for any arbitrary value of φ but on left-hand side, the term $\rho t\cos\varphi$ in the exponent suggests a dot product $\vec{\rho}\cdot\vec{t}$ with φ the angle between the vectors, while on the right-hand side, writing the harmonic-oscillator function $\Phi_{n,k}\left(\rho,\varphi;b\right)$ suggests that φ is the polar angle of the vector $\vec{\rho}$. To lift this apparent ambiguity, we introduce the polar angle φ_t of vector $\vec{t}$ explicitly by noting that if θ is the angle between vectors $\vec{\rho}$ and $\vec{t}$ with $\theta = \varphi - \varphi_t$, then according to Eq. (4)

$$\Phi_{n,k}\left(\rho,\theta;b\right) = \Phi_{n,|k|}\left(\rho;b\right) \frac{e^{ik\theta}}{\sqrt{2\pi}}$$

and therefore

$$\Phi_{n,k}\left(\rho,\theta;b\right) = \Phi_{n,k}\left(\rho,\varphi;b\right) e^{-ik\varphi_t} \tag{A.8}$$

Writing the left-hand side of Eq. (A.2) in vector form, we now have

$$e^{-\vec{t}^2+2\vec{\rho}\cdot\vec{t}/b-\rho^2/\left(2b^2\right)} = b\sqrt{\pi}\sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty}\frac{(-1)^n\,t^{2n+|k|}}{\sqrt{n!\,(n+|k|)!}}e^{-ik\varphi_t}\Phi_{n,k}\left(\rho,\varphi;b\right)$$

For convenience, we introduce the function

$$\chi_{n,k}\left(\vec{t}\right) \equiv \frac{(-1)^n}{n!}t^{2n+|k|}e^{-ik\varphi_t} \tag{A.9}$$

which allows us to write the generating function for polar harmonic-oscillator functions as

$$e^{-\vec{t}^2+2\vec{\rho}\cdot\vec{t}/b-\rho^2/\left(2b^2\right)} = b^2\sqrt{\frac{\pi}{2}}\sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty}\mathcal{N}_{n,|k|}\chi_{n,k}\left(\vec{t}\right)\Phi_{n,k}\left(\rho,\varphi;b\right)$$

This form will be convenient for some derivations, and we will obtain useful properties of the function $\chi_{n,k}\left(\vec{t}\right)$ in section A.5.

A.3 Polar-to-Cartesian mapping

Having derived generating functions for the harmonic-oscillator functions in both polar and Cartesian coordinates, we can now obtain a relation between the two,

$$\boxed{\Phi_{n_x}\left(x;b\right)\Phi_{n_y}\left(y;b\right) = \sum_{k=-n_x-n_y,2}^{n_x+n_y} C_{n,k}^{n_x,n_y}\Phi_{\frac{n_x+n_y-|k|}{2},k}\left(\rho,\varphi;b\right)} \tag{A.10}$$

where the coefficients $C_{n,k}^{n_x,n_y}$ are given by Eq. (A.17).

In order to relate the polar and Cartesian harmonic-oscillator functions we will use Eqs. (A.1) and (A.2). We will assume axial symmetry and use the same parameter b for all the coordinates involved. Consider the arbitrary vectors $\vec{\rho} = x\hat{x} + y\hat{y}$ and $\vec{t} = t_x\hat{x} + t_y\hat{y}$ in the two-dimensional Cartesian coordinate system, with $\vec{\rho}\cdot\vec{t} = \rho t\cos\theta$. Note that we are using the symbol θ for the angle between vectors $\vec{\rho}$ and $\vec{t}$. We can write

$$e^{-t_x^2+2t_xx/b-x^2/\left(2b^2\right)}e^{-t_y^2+2t_yy-y^2/\left(2b^2\right)} = e^{-t^2+2\rho t\cos\theta/b-\rho^2/\left(2b^2\right)}$$

Using Eqs. (A.1) and (A.2), this can also be written as

$$
\begin{aligned}
& b\sqrt{\pi}\sum_{n_x=0}^{\infty}\sum_{n_y=0}^{\infty}\frac{2^{(n_x+n_y)/2}}{\sqrt{n_x!n_y!}}t_x^{n_x}t_y^{n_y}\Phi_{n_x}(x;b)\,\Phi_{n_y}(y;b) \\
&= b\sqrt{\pi}\sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty}\frac{(-1)^n\,t^{2n+|k|}}{\sqrt{n!\,(n+|k|)!}}\Phi_{n,k}(\rho,\theta;b) \qquad \text{(A.11)}
\end{aligned}
$$

We must now equate the terms on the left-hand side to those on the right-hand side. We would like to introduce the polar angle φ of the vector $\vec{\rho}$ instead of the angle θ between $\vec{\rho}$ and $\vec{t}$ in these expressions, because the final result should be completely independent of the choice of vector $\vec{t}$. Using Eq. (A.8), Eq. (A.11) becomes

$$
\begin{aligned}
& \sum_{n_x=0}^{\infty}\sum_{n_y=0}^{\infty}\frac{2^{(n_x+n_y)/2}}{\sqrt{n_x!n_y!}}\left(\frac{t_x}{b}\right)^{n_x}\left(\frac{t_y}{b}\right)^{n_y}\Phi_{n_x}(x;b)\,\Phi_{n_y}(y;b) \\
&= \sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty}\frac{(-1)^n}{\sqrt{n!\,(n+|k|)!}}\left(\frac{t}{b}\right)^{2n+|k|}e^{-ik\varphi_t}\Phi_{n,k}(\rho,\varphi;b) \qquad \text{(A.12)}
\end{aligned}
$$

All we have to do now is identify terms on the left- and right-hand sides. We can establish this correspondence by expressing t and φ_t in terms of t_x and t_y. To this end, we write

$$
t^{2n+|k|}e^{-ik\varphi_t} = t^{2n}\left(te^{-is_k\varphi_t}\right)^{|k|}
$$

where we have introduced the sign quantity

$$
s_k \equiv \begin{cases} 1 & k \geq 0 \\ -1 & k < 0 \end{cases} \qquad \text{(A.13)}
$$

Note that we can write

$$
\begin{aligned}
te^{-is_k\varphi_t} &= t\cos(s_k\varphi_t) - it\sin(s_k\varphi_t) \\
&= t\cos\varphi_t - is_k t\sin\varphi_t \\
&= t_x - is_k t_y
\end{aligned}
$$

where the second line follows because $s_k = \pm 1$. Thus we have

$$
\begin{aligned}
t^{2n+|k|}e^{-ik\varphi_t} &= \left(t_x^2+t_y^2\right)^n (t_x - is_k t_y)^{|k|} \\
&= \sum_{p=0}^{n}\sum_{q=0}^{|k|}\begin{pmatrix} n \\ p \end{pmatrix}\begin{pmatrix} |k| \\ q \end{pmatrix}(-is_k)^{|k|-q}\,t_x^{2p+q}t_y^{2n+|k|-2p-q}
\end{aligned}
$$

We substitute this result into the right-hand side of Eq. (A.12) to get

$$RHS = \sum_{k=-\infty}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^n}{\sqrt{n!\,(n+|k|)!}} \left[\sum_{p=0}^{n} \sum_{q=0}^{|k|} \binom{n}{p} \binom{|k|}{q} (-is_k)^{|k|-q} \right.$$
$$\left. \times t_x^{2p+q} t_y^{2n+|k|-2p-q} \right] \Phi_{n,k}(\rho, \varphi; b) \tag{A.14}$$

Comparing with the left-hand side of Eq. (A.12), we see that we will need to make the identifications

$$\begin{aligned} 2p + q &= n_x \\ 2n + |k| - 2p - q &= n_y \end{aligned}$$

which also implies the important relation

$$n_x + n_y = 2n + |k| \tag{A.15}$$

We wish to replace the sums in Eq. (A.14) over n and p with sums over n_x and n_y. Since $n_x = 2p+q$, it is clear that n_x will span the full range of integers starting with 0. Similarly, Eq. (A.15) implies that $n_y = 2n + |k| - n_x$ and for any n_x, there will always be a set of n and k values such that n_y spans the full range of integers from 0, independently of the value of index n_x. Thus we can make the substitution

$$\sum_{n=0}^{\infty} \sum_{p=0}^{n} \rightarrow \sum_{n_x=0}^{\infty} \sum_{n_y=0}^{\infty}$$

Next, we note that Eq. (A.15) can also be written as $2n = n_x + n_y - |k|$, and since $n \geq 0$, we must therefore have $|k| \leq n_x + n_y$. Finally, $2p = n_x - q$, and since $p \geq 0$, we conclude that $q \leq n_x$. Thus we can also make the substitution

$$\sum_{k=-\infty}^{\infty} \sum_{q=0}^{|k|} \rightarrow \sum_{k=-n_x-n_y}^{n_x+n_y} \sum_{q=0}^{\min(n_x,|k|)}$$

and Eq. (A.14) becomes

$$RHS = \sum_{n_x=0}^{\infty} \sum_{n_y=0}^{\infty} \left[\sum_{k=-n_x-n_y,2}^{n_x+n_y} \sum_{q=0}^{\min(n_x,|k|)} \frac{(-1)^{(n_x+n_y-|k|)/2} (-is_k)^{|k|-q}}{\sqrt{\frac{n_x+n_y-|k|}{2}!\,\frac{n_x+n_y+|k|}{2}!}} \right.$$
$$\left. \times \binom{\frac{n_x+n_y-|k|}{2}}{\frac{n_x-q}{2}} \binom{|k|}{q} \Phi_{\frac{n_x+n_y-|k|}{2},k}(\rho, \varphi; b) \right] t_x^{n_x} t_y^{n_y} \tag{A.16}$$

Note that in the sum over k, the index can be stepped by 2 units at a time, because of the restrictions imposed by the factorials. Comparing the left-hand side of Eq. (A.12), and its right-hand side given by Eq. (A.16), we deduce

$$\frac{2^{(n_x+n_y)/2}}{\sqrt{n_x!n_y!}}\Phi_{n_x}(x;b)\,\Phi_{n_y}(y;b) = \sum_{k=-n_x-n_y,2}^{n_x+n_y}\sum_{q=0}^{\min(n_x,|k|)}\frac{(-1)^{(n_x+n_y-|k|)/2}(-is_k)^{|k|-q}}{\sqrt{\frac{n_x+n_y-|k|}{2}!\,\frac{n_x+n_y+|k|}{2}!}} \times \begin{pmatrix}\frac{n_x+n_y-|k|}{2}\\ \frac{n_x-q}{2}\end{pmatrix}\begin{pmatrix}|k|\\ q\end{pmatrix}\Phi_{\frac{n_x+n_y-|k|}{2},k}(\rho,\varphi;b)$$

or, in more compact notation,

$$\Phi_{n_x}(x;b)\,\Phi_{n_y}(y;b) = \sum_{k=-n_x-n_y,2}^{n_x+n_y} C_{n,k}^{n_x,n_y}\,\Phi_{\frac{n_x+n_y-|k|}{2},k}(\rho,\varphi;b)$$

where

$$\boxed{C_{n,k}^{n_x,n_y} \equiv \frac{\sqrt{n_x!n_y!}}{2^{(n_x+n_y)/2}}\frac{(-1)^{(n_x+n_y-|k|)/2}}{\sqrt{\frac{n_x+n_y-|k|}{2}!\,\frac{n_x+n_y+|k|}{2}!}}\sum_{q=0}^{\min(n_x,|k|)}(-is_k)^{|k|-q}\begin{pmatrix}\frac{n_x+n_y-|k|}{2}\\ \frac{n_x-q}{2}\end{pmatrix}\begin{pmatrix}|k|\\ q\end{pmatrix}} \tag{A.17}$$

The appearance of the index n in the symbol $C_{n,k}^{n_x,n_y}$, even though it is not explicitly used, serves as a reminder of the implicit relation between the indices given by Eq. (A.15).

A.4 Cartesian-to-polar mapping

In this section,we derive the inverse transformation corresponding to Eq. (A.10),

$$\boxed{\Phi_{n,k}(\rho,\varphi;b) = \sum_{n_y=0}^{2n+|k|} C_{n_x,n_y}^{n,k}\,\Phi_{2n+|k|-n_y}(x;b)\,\Phi_{n_y}(y;b)} \tag{A.18}$$

which expresses the polar harmonic-oscillator functions in terms of the Cartesian functions. The coefficients $C_{n_x,n_y}^{n,k}$ are given by Eq. (A.21).

We start again from Eq. (A.12), but this time, we express t_x and t_y on the left-hand side in terms of t and φ_t. Consider then

$$
\begin{aligned}
t_x^{n_x} t_y^{n_y} &= (t \cos\varphi_t)^{n_x} \, (t \sin\varphi_t)^{n_y} \\
&= t^{n_x+n_y} \left(\frac{e^{i\varphi_t} + e^{-i\varphi_t}}{2} \right)^{n_x} \left(\frac{e^{i\varphi_t} - e^{-i\varphi_t}}{2i} \right)^{n_y}
\end{aligned}
$$

Expanding the powers and grouping terms yields

$$
t_x^{n_x} t_y^{n_y} = \frac{t^{n_x+n_y}}{2^{n_x+n_y} i^{n_y}} \sum_{p=0}^{n_x} \sum_{q=0}^{n_y} \begin{pmatrix} n_x \\ p \end{pmatrix} \begin{pmatrix} n_y \\ q \end{pmatrix} (-1)^{n_y-q} \, e^{-i(n_x+n_y-2p-2q)\varphi_t}
$$

Substituting into the left-hand side of Eq. (A.12) produces

$$
\begin{aligned}
LHS = \sum_{n_x=0}^{\infty} \sum_{n_y=0}^{\infty} & \frac{t^{n_x+n_y}}{\sqrt{n_x! n_y!} 2^{(n_x+n_y)/2} i^{n_y}} \sum_{p=0}^{n_x} \sum_{q=0}^{n_y} \begin{pmatrix} n_x \\ p \end{pmatrix} \begin{pmatrix} n_y \\ q \end{pmatrix} (-1)^{n_y-q} \\
& \times e^{-i(n_x+n_y-2p-2q)\varphi_t} \Phi_{n_x}(x; b) \, \Phi_{n_y}(y; b)
\end{aligned}
$$

Comparing with the right-hand side of Eq. (A.12) we see that we need to make the identifications

$$
\begin{aligned}
n_x + n_y &= 2n + |k| && \text{(A.19)} \\
n_x + n_y - 2p - 2q &= k && \text{(A.20)}
\end{aligned}
$$

we therefore introduce a summation over n and k with the help of Kronecker-delta functions,

$$
\begin{aligned}
LHS = \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} & t^{2n+|k|} e^{-ik\varphi_t} 2^{-(n_x+n_y)/2} \sum_{n_x=0}^{\infty} \sum_{n_y=0}^{\infty} \delta_{n_x+n_y, 2n+|k|} \\
& \times \frac{\Phi_{n_x}(x; b) \, \Phi_{n_y}(y; b)}{\sqrt{n_x! n_y!} i^{n_y}} \sum_{p=0}^{n_x} \sum_{q=0}^{n_y} \delta_{2p+2q, n_x+n_y-k} \begin{pmatrix} n_x \\ p \end{pmatrix} \begin{pmatrix} n_y \\ q \end{pmatrix} (-1)^{n_y-q}
\end{aligned}
$$

where the Kronecker-delta functions collect those terms in the remaining summations needed to satisfy Eqs. (A.19) and (A.20). The restrictions imposed by the Kronecker-delta functions can be used to eliminate the summations over n_x and p

$$LHS = \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} t^{2n+|k|} e^{-ik\varphi_t} 2^{-n-|k|/2} \sum_{n_y=0}^{2n+|k|} \frac{\Phi_{2n+|k|-n_y}(x;b)\,\Phi_{n_y}(y;b)}{\sqrt{(2n+|k|-n_y)!n_y!}i^{n_y}}$$
$$\sum_{q=0}^{\min(n_y, n-q+(|k|-k)/2)} \binom{2n+|k|-n_y}{n-q+\frac{|k|-k}{2}} \binom{n_y}{q} (-1)^{n_y-q}$$

Comparing with the right-hand side of Eq. (A.12) we deduce the relation

$$2^{-n-|k|/2} \sum_{n_y=0}^{2n+|k|} \frac{\Phi_{2n+|k|-n_y}(x;b)\,\Phi_{n_y}(y;b)}{\sqrt{(2n+|k|-n_y)!n_y!}i^{n_y}}$$
$$\times \sum_{q=0}^{q_{max}} \binom{2n+|k|-n_y}{n-q+\frac{|k|-k}{2}} \binom{n_y}{q} (-1)^{n_y-q} = \frac{(-1)^n}{\sqrt{n!\,(n+|k|)!}} \Phi_{n,k}(\rho,\varphi;b)$$

where

$$q_{max} \equiv \min\left(n_y, n + (|k|-k)/2\right)$$

which we write as

$$\Phi_{n,k}(\rho,\varphi;b) = \sum_{n_y=0}^{2n+|k|} C^{n,k}_{n_x,n_y} \Phi_{2n+|k|-n_y}(x;b)\,\Phi_{n_y}(y;b)$$

with

$$\boxed{C^{n,k}_{n_x,n_y} = \frac{2^{-n-|k|/2}(-1)^n \sqrt{n!\,(n+|k|)!}}{\sqrt{(2n+|k|-n_y)!n_y!}i^{n_y}} \sum_{q=0}^{q_{max}} \binom{2n+|k|-n_y}{n-q+\frac{|k|-k}{2}} \binom{n_y}{q} (-1)^{n_y-q}} \tag{A.21}$$

The appearance of the index n_x in the symbol $C^{n,k}_{n_x,n_y}$, even though it is not explicitly used, serves as a reminder of the implicit relation between the indices given by Eq. (A.15).

A.5 Properties of the function $\chi_{n,k}\left(\vec{t}\right)$

In section A.2 we introduced the function $\chi_{n,k}\left(\vec{t}\right)$ which was used to obtain a generating function for harmonic-oscillator functions in polar coordinates. This function has many useful properties which we will exploit in further derivations. In this section, we obtain some important properties of $\chi_{n,k}\left(\vec{t}\right)$. From the definition of the $\chi_{n,k}\left(\vec{t}\right)$ function in Eq. (A.9),

$$\chi_{n,k}\left(\vec{t}\right) \equiv \frac{(-1)^n}{n!} t^{2n+|k|} e^{-ik\varphi_t}$$

we can easily show that

$$\boxed{t^{2m}\chi_{n,k}\left(\vec{t}\right) = (-1)^m \frac{(n+m)!}{n!}\chi_{n+m,k}\left(\vec{t}\right)} \tag{A.22}$$

As a corollary, we can use Eq. (A.22) to show

$$\boxed{e^{at^2}\chi_{n,k}\left(\vec{t}\right) = \sum_{m=0}^{\infty} \frac{(-a)^m (n+m)!}{m!n!}\chi_{n+m,k}\left(\vec{t}\right)} \tag{A.23}$$

The complex conjugate of $\chi_{n,k}\left(\vec{t}\right)$ is also readily expressed as

$$\boxed{\chi^*_{n,k}\left(\vec{t}\right) = \chi_{n,-k}\left(\vec{t}\right)} \tag{A.24}$$

and a scale factor can be factored out,

$$\boxed{\chi_{n,k}\left(a\vec{t}\right) = a^{2n+|k|}\chi_{n,k}\left(\vec{t}\right)} \tag{A.25}$$

Next, We will use the function $\chi_{n,k}$, to expand the expression $\exp\left(2\vec{t}_1 \cdot \vec{t}_2\right)$. Starting with the generating function for Bessel functions of the first kind, Eq. (A.6) with $z = -2it_1t_2$ and $\varphi = \varphi_1 - \varphi_2$,

$$e^{2\vec{t}_1\cdot\vec{t}_2} = \sum_{k=-\infty}^{\infty} i^{|k|} J_{|k|}\left(-2it_1t_2\right) e^{ik(\varphi_1-\varphi_2)} \tag{A.26}$$

Next, we use the series expansion for Bessel functions (Eq. 8.440 in [8]),

$$J_\nu\left(z\right) = \left(\frac{z}{2}\right)^\nu \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\left(\nu+k\right)!}\left(\frac{z}{2}\right)^{2k}$$

to write Eq. (A.26) as

$$
\begin{aligned}
e^{2\vec{t}_1\cdot\vec{t}_2} &= \sum_{k=-\infty}^{\infty} i^{|k|} e^{ik(\varphi_1-\varphi_2)} \left(-it_1t_2\right)^{|k|} \sum_{n=0}^{\infty} \frac{(-1)^n \left(-it_1t_2\right)^{2n}}{n!\,(|k|+n)!} \\
&= \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} \frac{1}{n!\,(|k|+n)!} \left(t_1t_2\right)^{2n+|k|} e^{ik(\varphi_1-\varphi_2)}
\end{aligned}
$$

or,

$$
\boxed{e^{2\vec{t}_1\cdot\vec{t}_2} = \frac{b^2}{2} \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} \mathcal{N}^2_{n,|k|}(b)\, \chi^*_{n,k}\left(\vec{t}_1\right) \chi_{n,k}\left(\vec{t}_2\right)} \tag{A.27}
$$

where $\mathcal{N}_{n_r,|\Lambda|}(b)$ is given by Eq. (6), and the oscillator parameter b cancels out in the right-hand side. Next, we derive an expression for the product of two $\chi_{n,k}$ functions, using the definition in Eq. (A.9)

$$
\chi_{n_1,k_1}\left(\vec{t}\right) \chi_{n_2,k_2}\left(\vec{t}\right) = \frac{(-1)^{n_1+n_2}}{n_1!n_2!} t^{2n_1+2n_2+|k_1|+|k_2|} e^{-i(k_1+k_2)\varphi_t} \tag{A.28}
$$

at this point, it is convenient to define the quantities

$$
n_{1,2} \equiv n_1 + n_2 + \frac{|k_1| + |k_2| - |k_1+k_2|}{2} \tag{A.29}
$$

$$
k_{1,2} \equiv \frac{|k_1| + |k_2| - |k_1+k_2|}{2} \tag{A.30}
$$

which recur throughout the paper. Then Eq. (A.28) becomes

$$
\chi_{n_1,k_1}\left(\vec{t}\right) \chi_{n_2,k_2}\left(\vec{t}\right) = (-1)^{-k_{1,2}} \frac{n_{1,2}!}{n_1!n_2!} \frac{(-1)^{n_{1,2}}}{n_{1,2}!} t^{2n_{1,2}+|k_1+k_2|} e^{-i(k_1+k_2)\varphi_t}
$$

or,

$$
\boxed{\chi_{n_1,k_1}\left(\vec{t}\right) \chi_{n_2,k_2}\left(\vec{t}\right) = (-1)^{k_{1,2}} \frac{n_{1,2}!}{n_1!n_2!} \chi_{n_{1,2},k_1+k_2}\left(\vec{t}\right)} \tag{A.31}
$$

Next, we obtain an expression for the function $\chi_{n,k}\left(\vec{t}_1+\vec{t}_2\right)$ of a sum of vectors. We write for an arbitrary vector $\vec{t}$

$$
e^{2\left(\vec{t}_1+\vec{t}_2\right)\cdot\vec{t}} = e^{2\vec{t}_1\cdot\vec{t}} e^{2\vec{t}_2\cdot\vec{t}} \tag{A.32}
$$

Using Eq. (A.27), the left-hand side is

$$
LHS = \frac{b^2}{2} \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} \mathcal{N}^2_{n,|k|}(b)\, \chi^*_{n,k}\left(\vec{t}_1+\vec{t}_2\right) \chi_{n,k}\left(\vec{t}\right) \tag{A.33}
$$

while the right-hand side of Eq. (A.32) is

$$RHS = \frac{b^4}{4} \sum_{n_1=0}^{\infty} \sum_{k_1=-\infty}^{\infty} \sum_{n_2=0}^{\infty} \sum_{k_2=-\infty}^{\infty} \mathcal{N}^2_{n_1,|k_1|}(b) \mathcal{N}^2_{n_2,|k_2|}(b)$$
$$\times \chi^*_{n_1,k_1}\left(\vec{t}_1\right) \chi^*_{n_2,k_2}\left(\vec{t}_2\right) \chi_{n_1,k_1}\left(\vec{t}\right) \chi_{n_2,k_2}\left(\vec{t}\right)$$

Using Eq. (A.31), this reduces to

$$RHS = \frac{b^4}{4} \sum_{n_1=0}^{\infty} \sum_{k_1=-\infty}^{\infty} \sum_{n_2=0}^{\infty} \sum_{k_2=-\infty}^{\infty} \mathcal{N}^2_{n_1,|k_1|}(b) \mathcal{N}^2_{n_2,|k_2|}(b) (-1)^{k_{1,2}} \frac{n_{1,2}!}{n_1! n_2!}$$
$$\times \chi^*_{n_1,k_1}\left(\vec{t}_1\right) \chi^*_{n_2,k_2}\left(\vec{t}_2\right) \chi_{n_{1,2},k_1+k_2}\left(\vec{t}\right)$$

In order to compare with Eq. (A.33), we introduce summations over the indices n and k with the help of Kronecker-delta functions,

$$RHS = \frac{b^4}{4} \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{n_1=0}^{\infty} \sum_{k_1=-\infty}^{\infty} \sum_{n_2=0}^{\infty} \sum_{k_2=-\infty}^{\infty} \mathcal{N}^2_{n_1,|k_1|}(b) \mathcal{N}^2_{n_2,|k_2|}(b) (-1)^{k_{1,2}} \frac{n_{1,2}!}{n_1! n_2!}$$
$$\times \chi^*_{n_1,k_1}\left(\vec{t}_1\right) \chi^*_{n_2,k_2}\left(\vec{t}_2\right) \delta_{n,n_{1,2}} \delta_{k,k_1+k_2} \chi_{n,k}\left(\vec{t}\right) \quad \text{(A.34)}$$

Comparing Eqs. (A.33) and (A.34) for an arbitrary vector $\vec{t}$, and taking the complex conjugate, we are lead to write

$$\boxed{\chi_{n,k}\left(\vec{t}_1 + \vec{t}_2\right) = \sum_{n_1=0}^{\infty} \sum_{k_1=-\infty}^{\infty} \sum_{n_2=0}^{\infty} \sum_{k_2=-\infty}^{\infty} D^{n,k}_{n_1,k_1;n_2,k_2} \chi_{n_1,k_1}\left(\vec{t}_1\right) \chi_{n_2,k_2}\left(\vec{t}_2\right)} \quad \text{(A.35)}$$

where

$$\boxed{D^{n,k}_{n_1,k_1;n_2,k_2} = (-1)^{n_1+n_2-n} \frac{(n+|k|)!}{(n_1+|k_1|)!\,(n_2+|k_2|)!} \delta_{n,n_{1,2}} \delta_{k,k_1+k_2}} \quad \text{(A.36)}$$

Note that we have used the condition imposed by the Kronecker-delta function $\delta_{n,n_{1,2}}$ and the definition of $n_{1,2}$ in Eq. (A.29) to write

$$(-1)^{k_{1,2}} = (-1)^{n_1+n_2-n}$$

Finally, we derive an expansion for the product $\exp\left(2\vec{t}_1 \cdot \vec{t}_2\right) \chi_{n,k}\left(\vec{t}_1 + \vec{t}_2\right)$. Though it is tempting to use Eq. (A.27) for this, we will adopt a different approach which will yield a simpler expression in the end. We write

$$e^{2\vec{t}_1\cdot\vec{t}_2/b^2}\chi_{n,k}\left(\vec{t}_1+\vec{t}_2\right)=e^{\left(\vec{t}_1+\vec{t}_2\right)^2}e^{-\left(t_1^2+t_2^2\right)}\chi_{n,k}\left(\vec{t}_1+\vec{t}_2\right)$$

We treat the first exponential on the right-hand side using Eq. (A.23), so that

$$e^{2\vec{t}_1\cdot\vec{t}_2}\chi_{n,k}\left(\vec{t}_1+\vec{t}_2\right)=e^{-\left(t_1^2+t_2^2\right)}\sum_{m=0}^{\infty}\frac{(-1)^m\,(n+m)!}{m!n!}\chi_{n+m,k}\left(\vec{t}_1+\vec{t}_2\right)$$

Next, we use Eq. (A.35) to expand the $\chi_{n+m,k}\left(\vec{t}_1+\vec{t}_2\right)$ function

$$\begin{aligned}e^{2\vec{t}_1\cdot\vec{t}_2}\chi_{n,k}\left(\vec{t}_1+\vec{t}_2\right)=e^{-\left(t_1^2+t_2^2\right)}&\sum_{m=0}^{\infty}\frac{(-1)^m\,(n+m)!}{m!n!}\\&\times\sum_{n_1=0}^{\infty}\sum_{k_1=-\infty}^{\infty}\sum_{n_2=0}^{\infty}\sum_{k_2=-\infty}^{\infty}D^{n+m,k}_{n_1,k_1;n_2,k_2}\\&\times\chi_{n_1,k_1}\left(\vec{t}_1\right)\chi_{n_2,k_2}\left(\vec{t}_2\right)\end{aligned}$$

and use Eq. (A.23) again to eliminate the remaining exponential on the right-hand side

$$\begin{aligned}e^{2\vec{t}_1\cdot\vec{t}_2}\chi_{n,k}\left(\vec{t}_1+\vec{t}_2\right)=&\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\sum_{n_1=0}^{\infty}\sum_{k_1=-\infty}^{\infty}\sum_{n_2=0}^{\infty}\sum_{k_2=-\infty}^{\infty}D^{n,k}_{n_1,k_1,m_1;n_2,k_2,m_2}\\&\times\chi_{n_1+m_1,k_1}\left(\vec{t}_1\right)\chi_{n_2+m_2,k_2}\left(\vec{t}_2\right)\end{aligned}\tag{A.37}$$

where we have defined

$$\begin{aligned}D^{n,k}_{n_1,k_1,m_1;n_2,k_2,m_2}\equiv&\sum_{m=0}^{\infty}\frac{(-1)^m\,(n+m)!\,(n_1+m_1)!\,(n_2+m_2)!}{m!n!m_1!n_1!m_2!n_2!}D^{n+m,k}_{n_1,k_1;n_2,k_2}\\=&\sum_{m=0}^{\infty}\frac{(-1)^{n_1+n_2-n}\,(n+m)!\,(n_1+m_1)!\,(n_2+m_2)!}{m!n!m_1!n_1!m_2!n_2!}\\&\times\frac{(n+m+|k|)!}{(n_1+|k_1|)!\,(n_2+|k_2|)!}\delta_{n+m,n_{1,2}}\delta_{k,k_1+k_2}\end{aligned}$$

which simplifies to

$$\begin{aligned}D^{n,k}_{n_1,k_1,m_1;n_2,k_2,m_2}\equiv&\frac{n_{1,2}!\,(n_1+m_1)!\,(n_2+m_2)!\,(n_{1,2}+|k_1+k_2|)!}{(n_{1,2}-n)!n!m_1!n_1!m_2!n_2!\,(n_1+|k_1|)!\,(n_2+|k_2|)!}\\&\times(-1)^{n_1+n_2-n}\,\delta_{n\le n_{1,2}}\delta_{k,k_1+k_2}\end{aligned}\tag{A.38}$$

Note the disappearance of the infinite sum over m in favor of the Kronecker-delta function $\delta_{n\le n_{1,2}}$.

B Decomposition of two-body Gaussian form

Consider the two-body Gaussian potential function in cylindrical coordinates

$$
\begin{aligned}
V(\vec{r}_1, \vec{r}_2) &= e^{-(\vec{r}_1 - \vec{r}_2)^2/\mu^2} \\
&= e^{-(\vec{\rho}_1 - \vec{\rho}_2)^2/\mu^2} e^{-(z_1 - z_2)^2/\mu^2}
\end{aligned}
$$

The critical first step in the separation method for harmonic-oscillator matrix elements is to write the potential itself in a form where the dependence on the coordinates $\vec{r}_1$ and $\vec{r}_2$ has been explicitly separated. We will therefore write this two-body function as a sum of one-body functions in the two coordinates. Note that the resulting sum will contain and infinite number of terms, while the matrix elements of the potential will be limited to a finite sum, thanks to properties of the harmonic-oscillator functions.

B.1 Cartesian component

The radial and Cartesian components of the potential can be expanded independently. We begin with the Cartesian term and postulate

$$
\begin{aligned}
V(z_1, z_2) &= e^{-(z_1 - z_2)^2/\mu^2} \\
&\equiv \sum_{n_z=0}^{\infty} f_{n_z}(z_1; b_z)\, \hat{\Phi}_{n_z}(z_2; b_z)
\end{aligned}
$$

choosing for the expansion the functions

$$
\boxed{\hat{\Phi}_{n_z}(z; b_z) \equiv e^{z^2/\left(2b_z^2\right)} \Phi_{n_z}(z; b_z)} \tag{B.1}
$$

We will now show that

$$
\boxed{f_{n_z}(z_1; b_z) = K_z^{1/2} \lambda_{n_z} e^{-z_1^2/\left(2G_z b_z^2\right)} \Phi_{n_z}\left(z_1; G_z^{1/2} b_z\right)} \tag{B.2}
$$

where the coefficients K_z and λ_{n_z} are given by Eqs. (B.5) and (B.6), respectively.

The exponential function in z^2 in front of the harmonic-oscillator function on the left-hand side has been added for computational convenience, as we shall see. Then, by orthogonality of the harmonic-oscillator functions, we have

$$\int_{-\infty}^{\infty} dz_2 e^{-z_2^2/\left(2b_z^2\right)} \Phi_{n_z}\left(z_2; b_z\right) V\left(z_1, z_2\right) = \int_{-\infty}^{\infty} dz_2 e^{-z_2^2/\left(2b_z^2\right)} \Phi_{n_z}\left(z_2; b_z\right) \times \left[\sum_{n'_z=0}^{\infty} f_{n'_z}\left(z_1; b_z\right) \hat{\Phi}_{n'_z}\left(z_2; b_z\right)\right] = f_{n_z}\left(z_1; b_z\right)$$

from which we obtain an explicit expression for the weight function $f_{n_z}\left(z_1; b_z\right)$,

$$\begin{aligned} f_{n_z}\left(z_1; b_z\right) &= \int_{-\infty}^{\infty} dz_2 e^{-z_2^2/\left(2b_z^2\right)} \Phi_{n_z}\left(z_2; b_z\right) V\left(z_1, z_2\right) \\ &= \mathcal{N}_{n_z} \int_{-\infty}^{\infty} dz_2 e^{-z_2^2/b_z^2} e^{-\left(z_1 - z_2\right)^2/\mu^2} H_{n_z}\left(\frac{z_2}{b_z}\right) \end{aligned} \tag{B.3}$$

Completing the square, we write

$$-\frac{z_2^2}{b_z^2} - \frac{\left(z_1 - z_2\right)^2}{\mu^2} = -\left[G_z^{1/2}\frac{z_2}{\mu} - G_z^{-1/2}\frac{z_1}{\mu}\right]^2 - \left(1 - \frac{1}{G_z}\right)\left(\frac{z_1}{\mu}\right)^2$$

where we have defined

$$G_z \equiv 1 + \frac{\mu^2}{b_z^2} \tag{B.4}$$

and the integral becomes

$$\begin{aligned} f_{n_z}\left(z_1; b_z\right) = &\mathcal{N}_{n_z} \exp\left[-\left(1 - \frac{1}{G_z}\right)\left(\frac{z_1}{\mu}\right)^2\right] \\ &\times \int_{-\infty}^{\infty} dz_2 \exp\left[-\left(G_z^{1/2}\frac{z_2}{\mu} - G_z^{-1/2}\frac{z_1}{\mu}\right)^2\right] H_{n_z}\left(\frac{z_2}{b_z}\right) \end{aligned}$$

Making the substitutions $x \equiv G_z^{1/2} z_2/\mu$, $y \equiv G_z^{-1/2} z_1/\mu$, $\alpha \equiv G_z^{-1/2}\mu/b_z$, the remaining integral can be evaluated using Eq. 7.374(8), p. 837 in [8],

$$\begin{aligned} f_{n_z}\left(z_1; b_z\right) = &\mu G_z^{-1/2} \mathcal{N}_{n_z} \pi^{1/2} \left(1 - \alpha^2\right)^{n_z/2} \exp\left[-\left(G_z - 1\right) y^2\right] \\ &\times H_{n_z}\left(\frac{\alpha y}{\sqrt{1 - \alpha^2}}\right) \end{aligned}$$

After some straightforward algebra and re-grouping of terms, this can be written as

$$
\begin{aligned}
f_{n_z}\left(z_1;b_z\right)= & \pi^{1/2}\mu G_z^{-1/2}G_z^{-n_z/2}e^{-z_1^2/\left(2G_zb_z^2\right)}G_z^{1/4} \\
& \times\left[\frac{1}{G_z^{1/4}}\mathcal{N}_{n_z}e^{-z_1^2/\left(2G_zb_z^2\right)}H_{n_z}\left(\frac{z_1}{G_z^{1/2}b_z}\right)\right]
\end{aligned}
$$

or, identifying the term in the square brackets with a harmonic-oscillator function with parameter $G_z^{1/2}b_z$ (note the extra factor $G_z^{1/4}$ needed to get the proper normalization constant $\mathcal{N}_{n_z}\left(G_z^{1/2}b_z\right)$),

$$
f_{n_z}\left(z_1;b_z\right)=K_z^{1/2}\lambda_{n_z}e^{-z_1^2/\left(2G_zb_z^2\right)}\Phi_{n_z}\left(z_1;G_z^{1/2}b_z\right)
$$

where

$$
K_z\equiv\frac{\pi\mu^2}{G_z^{1/2}} \tag{B.5}
$$

$$
\lambda_{n_z}\equiv G_z^{-n_z/2} \tag{B.6}
$$

B.2 Radial component

For the radial component of the Gaussian potential, we write

$$
\begin{aligned}
V\left(\vec{\rho}_1,\vec{\rho}_2\right)= & e^{-(\vec{\rho}_1-\vec{\rho}_2)^2/\mu^2} \\
\equiv & \sum_{n_r=0}^{\infty}\sum_{\Lambda=-\infty}^{\infty}f_{n_r,\Lambda}\left(\rho_1,\varphi_1;b_\perp\right)\hat{\Phi}_{n_r,\Lambda}\left(\rho_2,\varphi_2;b_\perp\right)
\end{aligned}
$$

where we have chosen

$$
\boxed{\hat{\Phi}_{n_r,\Lambda}\left(\rho,\varphi;b_\perp\right)\equiv e^{\frac{\rho^2}{2b_\perp^2}}\Phi_{n_r,\Lambda}\left(\rho,\varphi;b_\perp\right)} \tag{B.7}
$$

We will then show that

$$
\boxed{f_{n_r,\Lambda}\left(\rho_1,\varphi_1;b_\perp\right)=K_\perp\lambda_{2n_r+|\Lambda|}e^{-\rho_1^2/\left(2G_\perp b_\perp^2\right)}\Phi_{n_r,\Lambda}\left(\rho_1,\varphi_1;G_\perp^{1/2}b_\perp\right)} \tag{B.8}
$$

where the coefficients $K_\perp$ and $\lambda_{2n_r+|\Lambda|}$ are given by Eqs. (B.11) and (B.12), respectively.

By orthogonality of the harmonic-oscillator function we then have

$$
f_{n_r,\Lambda}\left(\rho_1,\varphi_1;b_\perp\right)=\int_0^\infty\rho_2d\rho_2\int_0^{2\pi}d\varphi_2e^{-\frac{\rho_2^2}{2b_\perp^2}}e^{-(\vec{\rho}_1-\vec{\rho}_2)^2/\mu^2}\Phi_{n_r,\Lambda}\left(\rho_2,\varphi_2;b_\perp\right)
$$

This integral can be evaluated in a straightforward way by transforming to a Cartesian coordinate system, and using Eq. (A.18),

$$
\begin{aligned}
f_{n_r,\Lambda}(\rho_1,\varphi_1;b_\perp) &= \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dy_2 e^{-\frac{x_2^2+y_2^2}{2b_\perp^2}} e^{-(x_1-x_2)^2/\mu^2-(y_1-y_2)^2/\mu^2} \\
&\quad \times \sum_{n_y=0}^{2n_r+|\Lambda|} C_{n_x,n_y}^{n_r,\Lambda} \Phi_{2n_r+|\Lambda|-n_y}(x_2;b_\perp)\, \Phi_{n_y}(y_2;b_\perp) \\
&= \sum_{n_y=0}^{2n_r+|\Lambda|} C_{n_x,n_y}^{n_r,\Lambda} \left[\int_{-\infty}^{\infty} dx_2 e^{-\frac{x_2^2}{2b_\perp^2}} e^{-(x_1-x_2)^2/\mu^2} \Phi_{2n_r+|\Lambda|-n_y}(x_2;b_\perp)\right] \\
&\quad \times \left[\int_{-\infty}^{\infty} dy_2 e^{-\frac{y_2^2}{2b_\perp^2}} e^{-(y_1-y_2)^2/\mu^2} \Phi_{n_y}(y_2;b_\perp)\right]
\end{aligned}
$$

The integrals in the square brackets are precisely those appearing in Eq. (B.3), and they are given by Eq. (B.2)

$$
\begin{aligned}
f_{n_r,\Lambda}(\rho_1,\varphi_1;b_\perp) = \sum_{n_y=0}^{2n_r+|\Lambda|} C_{n_x,n_y}^{n_r,\Lambda} & \Big[K_\perp^{1/2} \lambda_{2n_r+|\Lambda|-n_y} e^{-x_1^2/\left(2G_\perp b_\perp^2\right)} \\
& \Phi_{2n_r+|\Lambda|-n_y}\left(x_1; G_\perp^{1/2} b_\perp\right)\Big] \\
& \left[K_\perp^{1/2} \lambda_{n_y} e^{-y_1^2/\left(2G_\perp b_\perp^2\right)} \Phi_{n_y}\left(y_1; G_\perp^{1/2} b_\perp\right)\right]
\end{aligned}
\tag{B.9}
$$

where

$$G_\perp \equiv 1 + \frac{\mu^2}{b_\perp^2} \tag{B.10}$$

$$K_\perp \equiv \frac{\pi\mu^2}{G_\perp^{1/2}} \tag{B.11}$$

$$\lambda_n \equiv G_\perp^{-n/2} \tag{B.12}$$

and Eq. (B.9) can be further reduced to

$$
\begin{aligned}
f_{n_r,\Lambda}(\rho_1,\varphi_1;b_\perp) = K_\perp \lambda_{2n_r+|\Lambda|} & e^{-\rho_1^2/\left(2G_\perp b_\perp^2\right)} \\
& \sum_{n_y=0}^{2n_r+|\Lambda|} C_{n_x,n_y}^{n_r,\Lambda} \Phi_{2n_r+|\Lambda|-n_y}\left(x_1; G_\perp^{1/2} b_\perp\right) \Phi_{n_y}\left(y_1; G_\perp^{1/2} b_\perp\right)
\end{aligned}
$$

Finally, using Eq. (A.18) again to return to polar coordinates, we get

$$f_{n_r,\Lambda}(\rho_1,\varphi_1;b_\perp) = K_\perp \lambda_{2n_r+|\Lambda|} e^{-\rho_1^2/\left(2G_\perp b_\perp^2\right)} \Phi_{n_r,\Lambda}\left(\rho_1,\varphi_1; G_\perp^{1/2} b_\perp\right)$$

C Product of harmonic-oscillator functions

In this section, we will express the product of two harmonic-oscillator functions in terms of a sum of single oscillator functions. These results will be particularly useful in evaluating integrals where the integrand includes products of harmonic-oscillator functions.

C.1 Product of Cartesian harmonic-oscillator functions

In this section, we derive the form

$$\boxed{\Phi_{k_1}(x;b)\,\Phi_{k_2}(x;b) = \frac{e^{-x^2/\left(2b^2\right)}}{\sqrt{b\sqrt{\pi}}}\sum_{k=|k_1-k_2|,2}^{k_1+k_2} T^k_{k_1,k_2}\Phi_k(x;b)} \tag{C.1}$$

for the Cartesian harmonic-oscillator functions of Eq. (7), with the coefficients $T^k_{k_1,k_2}$ given by Eq. (C.6).

Using the generating function in Eq. (A.1), we write for any arbitrary variables t_1 and t_2,

$$\begin{aligned}
& e^{-t_1^2+2t_1x/b-x^2/\left(2b^2\right)}e^{-t_2^2+2t_2x/b-x^2/\left(2b^2\right)} \\
&= \left[\sqrt{b\sqrt{\pi}}\sum_{k_1=0}^{\infty}\frac{2^{k_1/2}}{\sqrt{k_1!}}t_1^{k_1}\Phi_{k_1}(x;b)\right] \\
&\quad\times\left[\sqrt{b\sqrt{\pi}}\sum_{k_2=0}^{\infty}\frac{2^{k_2/2}}{\sqrt{k_2!}}t_2^{k_2}\Phi_{k_2}(x;b)\right]
\end{aligned} \tag{C.2}$$

With the intent of manipulating the left-hand side of this equation into a form similar to the left-hand side of Eq. (A.1), we write

$$\begin{aligned}
LHS &= e^{-t_1^2-t_2^2+2(t_1+t_2)x/b-x^2/b^2} \\
&= e^{-(t_1+t_2)^2+2(t_1+t_2)x/b-x^2/\left(2b^2\right)}e^{2t_1t_2-x^2/\left(2b^2\right)}
\end{aligned}$$

Using Eq. (A.1), this becomes

$$
\begin{aligned}
LHS &= e^{2t_1t_2 - x^2/\left(2b^2\right)}\sqrt{b\sqrt{\pi}}\sum_{k=0}^{\infty}\frac{2^{k/2}}{\sqrt{k!}}\left(t_1+t_2\right)^k\Phi_k\left(x;b\right)\\
&= \sqrt{b\sqrt{\pi}}e^{-x^2/\left(2b^2\right)}\sum_{k=0}^{\infty}\frac{2^{k/2}}{\sqrt{k!}}\Phi_k\left(x;b\right)\sum_{p=0}^{\infty}\frac{\left(2t_1t_2\right)^p}{p!}\\
&\quad\times\sum_{q=0}^{k}\begin{pmatrix}k\\q\end{pmatrix}t_1^q t_2^{k-q}\\
&= \sqrt{b\sqrt{\pi}}e^{-x^2/\left(2b^2\right)}\sum_{k=0}^{\infty}\frac{2^{k/2}}{\sqrt{k!}}\Phi_k\left(x;b\right)\\
&\quad\times\sum_{q=0}^{k}\begin{pmatrix}k\\q\end{pmatrix}\sum_{p=0}^{\infty}\frac{2^p}{p!}t_1^{q+p}t_2^{k+p-q}
\end{aligned}
\tag{C.3}
$$

We can also group the terms in the right-hand side of Eq. (C.2),

$$
RHS = b\sqrt{\pi}\sum_{k_1=0}^{\infty}\sum_{k_2=0}^{\infty}\frac{2^{\left(k_1+k_2\right)/2}}{\sqrt{k_1!k_2!}}t_1^{k_1}t_2^{k_2}\Phi_{k_1}\left(x;b\right)\Phi_{k_2}\left(x;b\right)
\tag{C.4}
$$

Now we equate powers of t_1 and t_2 between Eqs. (C.3) and (C.4). We find that we must make the identifications

$$
\begin{aligned}
q+p &= k_1\\
k+p-q &= k_2
\end{aligned}
$$

which lead to

$$
\begin{aligned}
p &= \left(k_1+k_2-k\right)/2\\
q &= \left(k_1-k_2+k\right)/2
\end{aligned}
$$

so that Eq. (C.3) can be written

$$
\begin{aligned}
LHS &= \sqrt{b\sqrt{\pi}}e^{-x^2/\left(2b^2\right)}\sum_{k=\left|k_1-k_2\right|,2}^{k_1+k_2}\frac{2^{k/2}}{\sqrt{k!}}\Phi_k\left(x;b\right)\\
&\quad\times\sum_{k_1=0}^{\infty}\sum_{k_2=0}^{\infty}\begin{pmatrix}k\\\frac{k_1-k_2+k}{2}\end{pmatrix}\frac{2^{\left(k_1+k_2-k\right)/2}}{\left(\frac{k_1+k_2-k}{2}\right)!}t_1^{k_1}t_2^{k_2}
\end{aligned}
\tag{C.5}
$$

Note that the limits and step size for the summation over k are dictated by the need to keep the arguments of the factorials non-negative. In particular, the "2" appearing in the lower limit of the sum over k indicates that the index should be incremented by steps of 2. Direct comparison of Eqs. (C.4) and (C.5) now yields

$$\sqrt{b\sqrt{\pi}}e^{-x^2/\left(2b^2\right)} \sum_{k=|k_1-k_2|,2}^{k_1+k_2} \frac{2^{(k_1+k_2)/2}\sqrt{k!}}{\left(\frac{k_1-k_2+k}{2}\right)!\left(\frac{k_2-k_1+k}{2}\right)!\left(\frac{k_1+k_2-k}{2}\right)!}\Phi_k\left(x;b\right)$$
$$= b\sqrt{\pi}\frac{2^{(k_1+k_2)/2}}{\sqrt{k_1!k_2!}}\Phi_{k_1}\left(x;b\right)\Phi_{k_2}\left(x;b\right)$$

which leads to

$$\Phi_{k_1}\left(x;b\right)\Phi_{k_2}\left(x;b\right) = \frac{e^{-x^2/\left(2b^2\right)}}{\sqrt{b\sqrt{\pi}}} \sum_{k=|k_1-k_2|,2}^{k_1+k_2} T^k_{k_1,k_2}\Phi_k\left(x;b\right)$$

where

$$\boxed{T^k_{k_1,k_2} \equiv \frac{\sqrt{k_1!k_2!k!}}{\left(\frac{k_1-k_2+k}{2}\right)!\left(\frac{k_2-k_1+k}{2}\right)!\left(\frac{k_1+k_2-k}{2}\right)!}} \tag{C.6}$$

C.2 Product of radial harmonic-oscillator functions

Here, we obtain the relation

$$\boxed{\Phi_{n_1,k_1}\left(\rho,\varphi;b\right)\Phi_{n_2,k_2}\left(\rho,\varphi;b\right) = \frac{e^{-\rho^2/\left(2b^2\right)}}{\sqrt{\pi}b}\sum_{n=0}^{n_{1,2}} T^{n,k_1+k_2}_{n_1,k_1;n_2,k_2}\Phi_{n,k_1+k_2}\left(\rho,\varphi;b\right)} \tag{C.7}$$

between the harmonic-oscillator functions in polar coordinates defined in Eq. (4). The expansion coefficients $T^{n,k_1+k_2}_{n_1,k_1;n_2,k_2}$ are defined by Eq. (C.9).

Starting from the generating function in Eq. (A.3), and for arbitrary vectors $\vec{t}_1$ and $\vec{t}_2$

$$\begin{aligned} & e^{-\vec{t}_1^2+2\vec{\rho}\cdot\vec{t}_1/b-\rho^2/\left(2b^2\right)}e^{-\vec{t}_2^2+2\vec{\rho}\cdot\vec{t}_2/b-\rho^2/\left(2b^2\right)} \\ &= \left[b^2\sqrt{\frac{\pi}{2}}\sum_{k_1=-\infty}^{\infty}\sum_{n_1=0}^{\infty}\mathcal{N}_{n_1,|k_1|}\chi_{n_1,k_1}\left(\vec{t}_1\right)\Phi_{n_1,k_1}\left(\rho,\varphi;b\right)\right] \\ &\times\left[b^2\sqrt{\frac{\pi}{2}}\sum_{k_2=-\infty}^{\infty}\sum_{n_2=0}^{\infty}\mathcal{N}_{n_2,|k_2|}\chi_{n_2,k_2}\left(\vec{t}_2\right)\Phi_{n_2,k_2}\left(\rho,\varphi;b\right)\right] \end{aligned} \tag{C.8}$$

The left-hand side can be written

$$LHS = e^{-\left(\vec{t}_1+\vec{t}_2\right)^2+2\vec{\rho}\cdot\left(\vec{t}_1+\vec{t}_2\right)/b-\rho^2/\left(2b^2\right)} e^{2\vec{t}_1\cdot\vec{t}_2-\rho^2/\left(2b^2\right)}$$

Using Eq. (A.3) again to expand the first exponential, we get

$$LHS = e^{2\vec{t}_1\cdot\vec{t}_2-\rho^2/\left(2b^2\right)} b^2\sqrt{\frac{\pi}{2}} \sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty} \mathcal{N}_{n,|k|}\chi_{n,k}\left(\vec{t}_1+\vec{t}_2\right)\Phi_{n,k}\left(\rho,\varphi;b\right)$$

and using Eq. (A.37) to absorb the remaining exponential,

$$\begin{aligned}LHS = {} & b^2\sqrt{\frac{\pi}{2}}e^{-\rho^2/\left(2b^2\right)} \sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty} \mathcal{N}_{n,|k|}\Phi_{n,k}\left(\rho,\varphi;b\right)\\ & \times\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\sum_{p_1=0}^{\infty}\sum_{k_1=-\infty}^{\infty}\sum_{p_2=0}^{\infty}\sum_{k_2=-\infty}^{\infty} D^{n,k}_{p_1,k_1,m_1;p_2,k_2,m_2}\\ & \times\chi_{p_1+m_1,k_1}\left(\vec{t}_1\right)\chi_{p_2+m_2,k_2}\left(\vec{t}_2\right)\end{aligned}$$

Comparing with the right-hand side of Eq. (C.8) for arbitrary vectors $\vec{t}_1$ and $\vec{t}_2$, we make the identifications

$$\begin{aligned}p_1+m_1 &= n_1\\ p_2+m_2 &= n_2\end{aligned}$$

and write the left-hand side as

$$\begin{aligned}LHS = {} & b^2\sqrt{\frac{\pi}{2}}e^{-\rho^2/\left(2b^2\right)} \sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty} \mathcal{N}_{n,|k|}\Phi_{n,k}\left(\rho,\varphi;b\right)\\ & \times\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\sum_{n_1=0}^{\infty}\sum_{k_1=-\infty}^{\infty}\sum_{n_2=0}^{\infty}\sum_{k_2=-\infty}^{\infty} D^{n,k}_{n_1-m_1,k_1,m_1;n_2-m_2,k_2,m_2}\\ & \times\chi_{n_1,k_1}\left(\vec{t}_1;b\right)\chi_{n_2,k_2}\left(\vec{t}_2;b\right)\end{aligned}$$

Comparing again with the right-hand side of Eq. (C.8), we readily deduce

$$\begin{aligned}& b^4\frac{\pi}{2}\mathcal{N}_{n_1,|k_1|}\mathcal{N}_{n_2,|k_2|}\Phi_{n_1,k_1}\left(\rho,\varphi;b\right)\Phi_{n_2,k_2}\left(\rho,\varphi;b\right)\\ = {} & b^2\sqrt{\frac{\pi}{2}}e^{-\rho^2/\left(2b^2\right)} \sum_{k=-\infty}^{\infty}\sum_{n=0}^{\infty} \mathcal{N}_{n,|k|}\Phi_{n,k}\left(\rho,\varphi;b\right)\\ & \times\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty} D^{n,k}_{n_1-m_1,k_1,m_1;n_2-m_2,k_2,m_2}\end{aligned}$$

The sum over k disappears because of the Kronecker-delta function inside the D coefficient in Eq. (A.38) restricting the value of k to k_1+k_2, and the sum over n is cut off at $n = n_{1,2}$, because of the other Kronecker-delta function in Eq. (A.38) restricting its value. Therefore,

$$\Phi_{n_1,k_1}\left(\rho,\varphi;b\right)\Phi_{n_2,k_2}\left(\rho,\varphi;b\right) = \frac{e^{-\rho^2/\left(2b^2\right)}}{b^2}\sqrt{\frac{2}{\pi}}\sum_{n=0}^{n_{1,2}}\frac{\mathcal{N}_{n,|k_1+k_2|}}{\mathcal{N}_{n_1,|k_1|}\mathcal{N}_{n_2,|k_2|}}$$
$$\times\left[\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}D^{n,k_1+k_2}_{n_1-m_1,k_1,m_1;n_2-m_2,k_2,m_2}\right]$$
$$\times\Phi_{n,k_1+k_2}\left(\rho,\varphi;b\right)$$

which we write as

$$\Phi_{n_1,k_1}\left(\rho,\varphi;b\right)\Phi_{n_2,k_2}\left(\rho,\varphi;b\right) = \frac{e^{-\rho^2/\left(2b^2\right)}}{\sqrt{\pi}b}\sum_{n=0}^{n_{1,2}}T^{n,k_1+k_2}_{n_1,k_1;n_2,k_2}\Phi_{n,k_1+k_2}\left(\rho,\varphi;b\right)$$

The coefficients $T^{n,k_1+k_2}_{n_1,k_1;n_2,k_2}$ are obtained from Eq. (A.38), being careful to make the substitutions $n_1 \to n_1 - m_1$ and $n_2 \to n_2 - m_2$ (and therefore, according to Eq. (A.29), $n_{1,2} \to n_{1,2} - m_1 - m_2$ as well). Then,

$$T^{n,k_1+k_2}_{n_1,k_1;n_2,k_2} = (-1)^{n_1+n_2-n}\sqrt{\frac{n!\left(n_1+|k_1|\right)!\left(n_2+|k_2|\right)!}{n_1!n_2!\left(n+|k_1+k_2|\right)!}}\sum_{m_1=0}^{n_1}\sum_{m_2=0}^{n_2}(-1)^{m_1+m_2}$$
$$\times\begin{pmatrix}n_1\\m_1\end{pmatrix}\begin{pmatrix}n_2\\m_2\end{pmatrix}\begin{pmatrix}n_{1,2}-m_1-m_2\\n\end{pmatrix}$$
$$\times\frac{\left(n_{1,2}+|k_1+k_2|-m_1-m_2\right)!}{\left(n_1+|k_1|-m_1\right)!\left(n_2+|k_2|-m_2\right)!}\delta_{n\leq n_{1,2}-m_1-m_2}$$

or, in more compact notation,

$$T^{n,k_1+k_2}_{n_1,k_1;n_2,k_2} = (-1)^{n_1+n_2-n}\sqrt{\frac{n!\left(n_1+|k_1|\right)!\left(n_2+|k_2|\right)!}{n_1!n_2!\left(n+|k_1+k_2|\right)!}}$$
$$\times\sum_{m_1=0}^{n_1}\sum_{m_2=0}^{n_2}\delta_{n\leq n_{1,2}-m_1-m_2}C^{n,k_1+k_2}_{n_1,k_1,m_1;n_2,k_2,m_2} \tag{C.9}$$

with

$$C_{n_1,k_1,m_1;n_2,k_2,m_2}^{n,k_1+k_2} \equiv (-1)^{m_1+m_2} \begin{pmatrix} n_1 \\ m_1 \end{pmatrix} \begin{pmatrix} n_2 \\ m_2 \end{pmatrix} \begin{pmatrix} n_{1,2} - m_1 - m_2 \\ n \end{pmatrix} \times \frac{(n_{1,2} + |k_1 + k_2| - m_1 - m_2)!}{(n_1 + |k_1| - m_1)!\,(n_2 + |k_2| - m_2)!} \tag{C.10}$$

Note again that the Kronecker-delta function $\delta_{n \leq n_{1,2} - m_1 - m_2}$ ensures that we always have $n \leq n_{1,2}$, which we used to limit the sum over n in Eq. (C.7).

D Formalism for large oscillator shell number

In this section, we derive the result in [9],

$$\langle n_1 | f_n | n_2 \rangle = \frac{\mu b^{-1/2}}{\sqrt{2}\pi^{5/2}} \frac{\Gamma(\xi - n_1)\,\Gamma(\xi - n_2)\,\Gamma(\xi - n)}{z^{\xi}\sqrt{n! n_1! n_2!}} \times {}_2F_1(-n_1, -n_2; -\xi + n + 1; 1 - z) \tag{D.1}$$

with ξ given by Eq. (D.6) and z by Eq. (D.10), for the numerically accurate calculation of the matrix element $\langle n_1 | f_n | n_2 \rangle$ in Eq. (12) when large oscillator-shell numbers are involved. Note that our result differs slightly from [9] in that a "$b^{-1/2}$" factors appears in Eq. (D.1) instead of "$b^{1/2}$" (see discussion at the end of this section). The formula in Eq. (D.1) is preferred to the one in Eq. (19) for large oscillator-shell numbers, because the latter requires the evaluation of a sum of products of large (T) and small ($\bar{I}$) coefficients, which can be numerically unstable. We also obtain the corresponding matrix elements in Eq. (10)

$$V_{ijkl}^{(z)} = \frac{\mu}{\sqrt{2\pi^3} b_z} \sum_{n_z = \left| n_z^{(j)} - n_z^{(l)} \right|, 2}^{n_z^{(j)} + n_z^{(l)}} T_{n_z^{(j)}, n_z^{(l)}}^{n_z} \bar{F}_{n_z^{(i)}, n_z^{(k)}}^{n_z} \tag{D.2}$$

where the coefficients $\bar{F}_{n_z^{(i)}, n_z^{(k)}}^{n_z}$ are defined by Eq. (D.12).

Starting from the definition,

$$\langle n_1 | f_n | n_2 \rangle = K_z^{1/2} \lambda_n \int_{-\infty}^{\infty} dz\, \Phi_{n_1}(z; b)\, e^{-z^2/\left(2Gb^2\right)} \Phi_n\left(z; G^{1/2} b\right) \Phi_{n_2}(z; b)$$

we use the generating function, Eq. (A.1), to integrate the product of three harmonic-oscillator functions with the Gaussian factor. This produces

$$e^{-t_1^2-t_2^2-t^2}\int_{-\infty}^{\infty} dz\, e^{2(t_1+t_2)z/b+2tz/B-\nu z^2}$$
$$= \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n=0}^{\infty} C_{n_1,n_2,n} t_1^{n_1} t_2^{n_2} t^n \left\langle n_1 \left| f_n \right| n_2 \right\rangle \tag{D.3}$$

where

$$B \equiv G^{1/2} b$$

$$\nu \equiv \frac{1}{b^2} + \frac{1}{B^2}$$

$$C_{n_1,n_2,n} \equiv \frac{b\sqrt{\pi}\sqrt{B\sqrt{\pi}}}{K_z^{1/2}\lambda_n} \frac{2^{(n_1+n_2+n)/2}}{\sqrt{n_1!}\sqrt{n_2!}\sqrt{n!}}$$

The integral in the left-hand side of Eq. (D.3) is easily evaluated by completing the square in the exponential, giving

$$LHS = \sqrt{\frac{\pi}{\nu}} e^{-t_1^2-t_2^2-t^2+\tau^2/\nu} \tag{D.4}$$

where

$$\tau \equiv \frac{t_1+t_2}{b} + \frac{t}{B}$$

After some simplification, Eq. (D.4) takes the form

$$LHS = \sqrt{\frac{\pi}{\nu}} \exp\left\{\left[\alpha\left(t_1+t_2\right)-t\right]^2 \zeta + 2t_1t_2\right\}$$

with

$$\alpha \equiv G^{-1/2}$$

$$\zeta \equiv -\frac{G}{G+1}$$

which we expand as a series

$$
\begin{aligned}
LHS &= \sqrt{\frac{\pi}{\nu}} \sum_{i=0}^{\infty} \frac{(2t_1 t_2)^i}{i!} \sum_{p=0}^{\infty} \frac{1}{p!} \left[\alpha\left(t_1 + t_2\right) - t\right]^{2p} \zeta^p \\
&= \sqrt{\frac{\pi}{\nu}} \sum_{i=0}^{\infty} \sum_{p=0}^{\infty} \sum_{q=0}^{2p} \sum_{s=0}^{2p-q} \frac{2^i}{p!i!} \begin{pmatrix} 2p \\ q \end{pmatrix} \begin{pmatrix} 2p-q \\ s \end{pmatrix} (-\alpha)^{2p-q} \zeta^p t_1^{s+i} t_2^{2p-q-s+i} t^q
\end{aligned}
$$

comparing with the right-hand side of Eq. (D.3), we make the identifications

$$
\begin{aligned}
s + i = n_1 &\Rightarrow s = n_1 - i \\
2p - q - s + i = n_2 &\Rightarrow p = \frac{n_1 + n_2 + q}{2} - i \\
q = n &
\end{aligned}
$$

Note that this implies $n_1 + n_2 + n$ must be even, and the summation over i terminates after a finite number of terms, although we will let it run up to ∞ for notational convenience, letting the factorial terms implicitly truncate the sum. Then we have

$$
\begin{aligned}
&C_{n_1,n_2,n} \left\langle n_1 \left| f_n \right| n_2 \right\rangle \\
&= \sqrt{\frac{\pi}{\nu}} (-\alpha)^{n_1+n_2} \zeta^{(n_1+n_2+n)/2} \\
&\quad \times \sum_{i=0}^{\infty} \frac{\begin{pmatrix} n_1 + n_2 + n - 2i \\ n \end{pmatrix} \begin{pmatrix} n_1 + n_2 - 2i \\ n_1 - i \end{pmatrix}}{\left(\frac{n_1+n_2+n}{2} - i\right)! i!} \left(\frac{2}{\alpha^2 \zeta}\right)^i \\
&= \sqrt{\frac{\pi}{\nu}} (-\alpha)^{n_1+n_2} \zeta^{(n_1+n_2+n)/2} \\
&\quad \times \sum_{i=0}^{\infty} \frac{(n_1 + n_2 + n - 2i)!}{n! (n_1 - i)! (n_2 - i)! \left(\frac{n_1+n_2+n}{2} - i\right)! i!} \left(\frac{2}{\alpha^2 \zeta}\right)^i
\end{aligned}
\tag{D.5}
$$

Next, we simplify the ratio of factorials

$$
\frac{(2p)!}{p!} = \frac{(n_1 + n_2 + n - 2i)!}{\left(\frac{n_1+n_2+n}{2} - i\right)!}
$$

using the doubling formula for the Gamma function (Eq. 8.335(1) in [8]),

$$
\frac{(2p)!}{p!} = \frac{2^{2p}}{\sqrt{\pi}} \Gamma\left(p + \frac{1}{2}\right)
$$

For convenience, we define

$$\xi \equiv \frac{n_1 + n_2 + n + 1}{2} \tag{D.6}$$

which is a half-integer since we have already noted that $n_1 + n_2 + n$ is even. Then $p = \xi - i - 1/2$, and

$$\frac{(2p)!}{p!} = \frac{2^{2p}}{\sqrt{\pi}} \Gamma(\xi - i) \tag{D.7}$$

In order to simplify this further, we derive the following useful identity

$$\begin{aligned}
\Gamma(1 - \xi + i) &= (i - \xi)\,\Gamma(i - \xi) \\
&= (i - \xi)(i - \xi - 1) \cdots (1 - \xi)\,\Gamma(1 - \xi) \\
&= (-1)^i (\xi - 1) \cdots (\xi - (i - 1))(\xi - i)\,\Gamma(1 - \xi)
\end{aligned}$$

Similarly, we can write

$$\Gamma(\xi) = (\xi - 1) \cdots (\xi - (i - 1))(\xi - i)\,\Gamma(\xi - i)$$

Therefore,

$$\Gamma(1 - \xi + i) = (-1)^i \frac{\Gamma(\xi)\,\Gamma(1 - \xi)}{\Gamma(\xi - i)} \tag{D.8}$$

and, equivalently,

$$\Gamma(\xi - i) = (-1)^i \frac{\Gamma(\xi)\,\Gamma(1 - \xi)}{\Gamma(1 - \xi + i)} \tag{D.9}$$

Thus, Eq. (D.7) becomes

$$\begin{aligned}
\frac{(2p)!}{p!} &= \frac{2^{2p}}{\sqrt{\pi}} (-1)^i \frac{\Gamma(\xi)\,\Gamma(1 - \xi)}{\Gamma(1 - \xi + i)} \\
&= \frac{2^{2p}}{\sqrt{\pi}} (-1)^i \frac{\Gamma(\xi)}{(1 - \xi)_i}
\end{aligned}$$

where we have used the Pochhammer symbol

$$(x)_n \equiv \frac{\Gamma(x + n)}{\Gamma(x)} = x(x + 1) \cdots (x + n - 1)$$

Returning to Eq. (D.5), we replace the $(n_1 - i)!$ and $(n_2 - i)!$ terms with Pochhammer symbols as well using Eq. (D.9) with $\xi \to n_1 + 1$ to write

$$\begin{aligned}(n_1-i)! &= \Gamma\left(n_1-i+1\right)\\ &= (-1)^i \frac{\Gamma\left(n_1+1\right)\Gamma\left(-n_1\right)}{\Gamma\left(-n_1+i\right)}\\ &= (-1)^i \frac{n_1!}{\left(-n_1\right)_i}\end{aligned}$$

and similarly for $(n_2-i)!$. Then, Eq. (D.5) yields

$$\langle n_1\left|f_n\right|n_2\rangle = \frac{2^{2\xi-1}\Gamma\left(\xi\right)\left(-\alpha\right)^{n_1+n_2}\zeta^{(n_1+n_2+n)/2}}{\sqrt{\nu}C_{n_1,n_2,n}n!n_1!n_2!}\sum_{i=0}^{\infty}\frac{\left(-n_1\right)_i\left(-n_2\right)_i}{\left(1-\xi\right)_i i!}\left(-\frac{1}{2\alpha^2\zeta}\right)^i$$

which we express as a hypergeometric function, as defined in [8] Eq. 9.100 (see also section 9.14(2) in [8] for the notation in terms of a generalized hypergeometric function),

$$\langle n_1\left|f_n\right|n_2\rangle = \frac{2^{\xi-1/2}\mu\Gamma\left(\xi\right)\left(-\alpha\right)^{n_1+n_2}\zeta^{(n_1+n_2+n)/2}}{\sqrt{\nu}b\sqrt{B\sqrt{\pi}}\sqrt{n!n_1!n_2!}G^{1/4}G^{n/2}}\,{}_2F_1\left(-n_1,-n_2;1-\xi;z\right)$$

where

$$z \equiv -\frac{1}{2\alpha^2\zeta} = 1+\frac{\mu^2}{2b^2} \tag{D.10}$$

Simplifying further, we find

$$\begin{aligned}\langle n_1\left|f_n\right|n_2\rangle &= (-1)^{(n_1+n_2-n)/2}\frac{\mu}{\sqrt{2b\sqrt{\pi}}}\frac{\Gamma\left(\xi\right)}{\sqrt{n!n_1!n_2!}}z^{-\xi}\\ &\quad\times{}_2F_1\left(-n_1,-n_2;1-\xi;z\right)\end{aligned} \tag{D.11}$$

Comparing with Eq. (3) in [9], we note that the hypergeometric function is evaluated at $1-z$ rather than z in that paper. In order to make a direct comparison with [9], we use Eq. 9.131(2) in [8],

$$\begin{aligned}&{}_2F_1\left(-n_1,-n_2;1-\xi;z\right)\\ &= \frac{\Gamma\left(1-\xi\right)\Gamma\left(1-\xi+n_1+n_2\right)}{\Gamma\left(1-\xi+n_1\right)\Gamma\left(1-\xi+n_2\right)}\,{}_2F_1\left(-n_1,-n_2;-n_1-n_2+\xi;1-z\right)\\ &\quad+(1-z)^{1-\xi+n_1+n_2}\frac{\Gamma\left(1-\xi\right)\Gamma\left(-n_1-n_2+\xi-1\right)}{\Gamma\left(-n_1\right)\Gamma\left(-n_2\right)}\\ &\quad\times{}_2F_1\left(1-\xi+n_1,1-\xi+n_2;2-\xi+n_1+n_2;1-z\right)\end{aligned}$$

The second term vanishes because of the Gamma functions with negative-integer (or zero) arguments in the denominator. We can simplify the third argument of the hypergeometric function in the first term to

$$\begin{aligned} -n_1 - n_2 + \xi &= \frac{-n_1 - n_2 + n + 1}{2} \\ &= -\xi + n + 1 \end{aligned}$$

Thus,

$$\begin{aligned} {}_2F_1\left(-n_1, -n_2; 1-\xi; z\right) &= \frac{\Gamma\left(1-\xi\right)\Gamma\left(\xi-n\right)}{\Gamma\left(1-\xi+n_1\right)\Gamma\left(1-\xi+n_2\right)} \\ &\quad \times {}_2F_1\left(-n_1, -n_2; -\xi+n+1; 1-z\right) \end{aligned}$$

Next, we use Eq. (D.8) to re-write the Gamma functions in the denominator,

$$\begin{aligned} {}_2F_1\left(-n_1, -n_2; 1-\xi; z\right) &= (-1)^{n_1+n_2} \frac{\Gamma\left(\xi-n_1\right)\Gamma\left(\xi-n_2\right)\Gamma\left(\xi-n\right)}{\Gamma\left(1-\xi\right)\Gamma\left(\xi\right)\Gamma\left(\xi\right)} \\ &\quad \times {}_2F_1\left(-n_1, -n_2; -\xi+n+1; 1-z\right) \end{aligned}$$

Substituting this expression into Eq. (D.11) gives

$$\begin{aligned} \langle n_1 \left| f_n \right| n_2 \rangle &= (-1)^{(-n_1-n_2-n)/2} \frac{\mu}{\sqrt{2b\sqrt{\pi}}} \frac{\Gamma\left(\xi-n_1\right)\Gamma\left(\xi-n_2\right)\Gamma\left(\xi-n\right)}{\sqrt{n!n_1!n_2!}\Gamma\left(1-\xi\right)\Gamma\left(\xi\right)} z^{-\xi} \\ &\quad \times {}_2F_1\left(-n_1, -n_2; -\xi+n+1; 1-z\right) \end{aligned}$$

Finally, we use Eq. 8.334(3) in [8] to write

$$\begin{aligned} \langle n_1 \left| f_n \right| n_2 \rangle &= (-1)^{(-n_1-n_2-n)/2} \frac{\mu}{\sqrt{2b\sqrt{\pi}}} \frac{\Gamma\left(\xi-n_1\right)\Gamma\left(\xi-n_2\right)\Gamma\left(\xi-n\right)}{\sqrt{n!n_1!n_2!}\pi\left(-1\right)^{(n_1+n_2+n)/2}} z^{-\xi} \\ &\quad \times {}_2F_1\left(-n_1, -n_2; -\xi+n+1; 1-z\right) \\ &= \frac{\mu b^{-1/2}}{\sqrt{2\pi^{5/2}}} \frac{\Gamma\left(\xi-n_1\right)\Gamma\left(\xi-n_2\right)\Gamma\left(\xi-n\right)}{z^{\xi}\sqrt{n!n_1!n_2!}} \\ &\quad \times {}_2F_1\left(-n_1, -n_2; -\xi+n+1; 1-z\right) \end{aligned}$$

This result is nearly identical to Eq. (3) in [9], after properly adjusting for the choice of variable names, the only minor difference being the oscillator parameter which appears as $b^{-1/2}$ in the present work, and $b^{1/2}$ in [9]. However, dimensional analysis favors the $b^{-1/2}$ form, as the matrix element $\langle n_1 \left| f_n \right| n_2 \rangle$ must carry dimensions of length to the $1/2$ power, according to its definition in

Eq. (12). In closing, we use Eq. (D.1) to write the expression for the two-body matrix element (corresponding to Eq. (10) in the large oscillator-shell limit),

$$V_{ijkl}^{(z)} = \frac{\mu}{\sqrt{2\pi^3} b_z} \sum_{n_z = \left| n_z^{(j)} - n_z^{(l)} \right|, 2}^{n_z^{(j)} + n_z^{(l)}} T^{n_z}_{n_z^{(j)}, n_z^{(l)}} \bar{F}^{n_z}_{n_z^{(i)}, n_z^{(k)}}$$

where

$$\begin{aligned} \bar{F}^{n_z}_{n_z^{(i)}, n_z^{(k)}} \equiv & \frac{\Gamma\left(\xi - n_z^{(i)}\right) \Gamma\left(\xi - n_z^{(k)}\right) \Gamma\left(\xi - n_z\right)}{z^{\xi} \sqrt{n_z! n_z^{(i)}! n_z^{(k)}!}} \\ & \times {}_2F_1\left(-n_z^{(i)}, -n_z^{(k)}; -\xi + n_z + 1; 1 - z\right) \end{aligned} \tag{D.12}$$

E Angular integral

We wish to evaluate the radial part of the matrix-element integral

$$\begin{aligned} V_{ijkl}^{(r)} \equiv & \int_0^{\infty} \rho_1 d\rho_1 \int_0^{2\pi} d\varphi_1 \int_0^{\infty} \rho_2 d\rho_2 \int_0^{2\pi} d\varphi_2 \\ & \times \Phi^*_{n_r^{(i)}, \Lambda^{(i)}} \left(\rho_1, \varphi_1; b_\perp\right) \Phi^*_{n_r^{(j)}, \Lambda^{(j)}} \left(\rho_2, \varphi_2; b_\perp\right) \\ & \times e^{-(\vec{\rho}_1 - \vec{\rho}_2)^2/\mu^2} \Phi_{n_r^{(k)}, \Lambda^{(k)}} \left(\rho_1, \varphi_1; b_\perp\right) \Phi_{n_r^{(l)}, \Lambda^{(l)}} \left(\rho_2, \varphi_2; b_\perp\right) \end{aligned}$$

numerically, where the harmonic-oscillator functions are defined in Eq. (4). By rotational invariance of the Gaussian potential, we have

$$-\Lambda^{(i)} - \Lambda^{(j)} + \Lambda^{(k)} + \Lambda^{(l)} = 0$$

The angular integrals over φ_1 and φ_2 are particularly problematic because of their oscillatory nature. Therefore, we focus on those integrals and introduce the function

$$\Theta_k\left(x\right) \equiv \frac{1}{\left(2\pi\right)^2} \int_0^{2\pi} d\varphi_1 \int_0^{2\pi} d\varphi_2 e^{ik(\varphi_1 - \varphi_2)} e^{2x \cos(\varphi_1 - \varphi_2)} \tag{E.1}$$

so that we may write

$$V_{ijkl}^{(r)} = \int_0^\infty \rho_1 d\rho_1 \int_0^\infty \rho_2 d\rho_2 e^{-\left(\rho_1^2+\rho_2^2\right)/\mu^2} \Phi_{n_r^{(i)},\left|\Lambda^{(i)}\right|}\left(\rho_1; b_\perp\right) \Phi_{n_r^{(j)},\left|\Lambda^{(j)}\right|}\left(\rho_2; b_\perp\right)$$
$$\Phi_{n_r^{(k)},\left|\Lambda^{(k)}\right|}\left(\rho_1; b_\perp\right) \Phi_{n_r^{(l)},\left|\Lambda^{(l)}\right|}\left(\rho_2; b_\perp\right) \Theta_{-\Lambda^{(i)}+\Lambda^{(k)}}\left(\frac{\rho_1\rho_2}{\mu^2}\right) \tag{E.2}$$

We simplify Eq. (E.1) using the generating function for the Bessel function, given in Eq. (A.6), with $z = -2ix$ and $\varphi = \varphi_1 - \varphi_2$,

$$e^{2x\cos(\varphi_1-\varphi_2)} = \sum_{n=-\infty}^{\infty} i^{|n|} J_{|n|}\left(-2ix\right) e^{in(\varphi_1-\varphi_2)}$$

from which the integral in Eq. (E.1) yields

$$\Theta_k\left(x\right) = i^{|k|} J_{|k|}\left(-2ix\right)$$

From the series expansion of the modified Bessel function of the first kind, Eq. 8.445 in [8], we get

$$\begin{aligned}\Theta_k\left(x\right) &= (-1)^{|k|} I_{|k|}\left(-2x\right)\\ &= \sum_{n=0}^{\infty} \frac{x^{2n}}{n!\left(n+|k|\right)!}\end{aligned} \tag{E.3}$$

We find that the series in Eq. (E.3) is extremely well converged if we include terms up to m such that

$$\left|\frac{x^{2m}}{m!\left(m+|k|\right)!}\right| < \epsilon$$

where $\epsilon = 10^{-2N_0-N_{\text{quad}}/8}$ for a calculation in up to N_0 oscillator shells and N_{quad} quadrature points. The remaining integrals over ρ_1 and ρ_2 in Eq. (E.2) were evaluated by Gauss-Laguerre quadrature.

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